Electronic Supplementary Material (ESI) for ChemComm.


# Electronic Supplementary Information For

# Energetic Performance of Trinitromethyl Nitrotriazole (TNMNT)

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**Table S1.** Calculated Total Energy ($E_0$), Zero-point Energy (ZPE), values of Thermal Correction ($H_T$) and Enthalpy of Formation ($\Delta H_f°$ (g)) of the title compounds using B3LYP/6-31+G**//MP2/6-311++G** level of theory (Isodesmic).

| Compounds | $E_0$ [Hartree/Particle] | ZPE [Hartree/Particle] | $H_T$ [Hartree/Particle] | $\Delta H_f°$ (g) kJ/mol | $\Delta H_{sub}°$ kJ/mol | $\Delta H_f°$ (s) kJ/mol |
|---|---|---|---|---|---|---|
| **$CH_3$-$NH_2$** | -95.5938424 | 0.064026 | 0.004375 | -23.00[a] | ---- | ---- |
| **MNTri** | -484.9528302 | 0.089889 | 0.008602 | 177.14[b] | ---- | ---- |
| **TNMA** | -707.8916215 | 0.070293 | 0.011293 | -45.04[b] | ---- | ---- |
| **DNMA-anion** | -503.1473114 | 0.056419 | 0.008260 | -215.20[b] | ---- | ---- |
| **6** | -1097.209992 | 0.094711 | 0.016221 | 155.10[c] | 70.31 | 84.79 |
| **9-10 anion** | | | | -15.06[c] | | |
| **9($NH_3NH_2$)** | ---- | ---- | ---- | 754.94[c] | 489.83[d] | 265.11 |
| **10($K^+$)** | ---- | ---- | ---- | 486.04[c] | 498.48[d] | -12.44 |

[a] 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.] [b]Obtained at G2 level. [c]Calculated using isodesmic equation as shown in Figure S1.

The gas-phase enthalpies of formation $\Delta_f H°(g)$ were predicted using Gaussian 03 program[1] based on isodesmic equations (Figure S1).

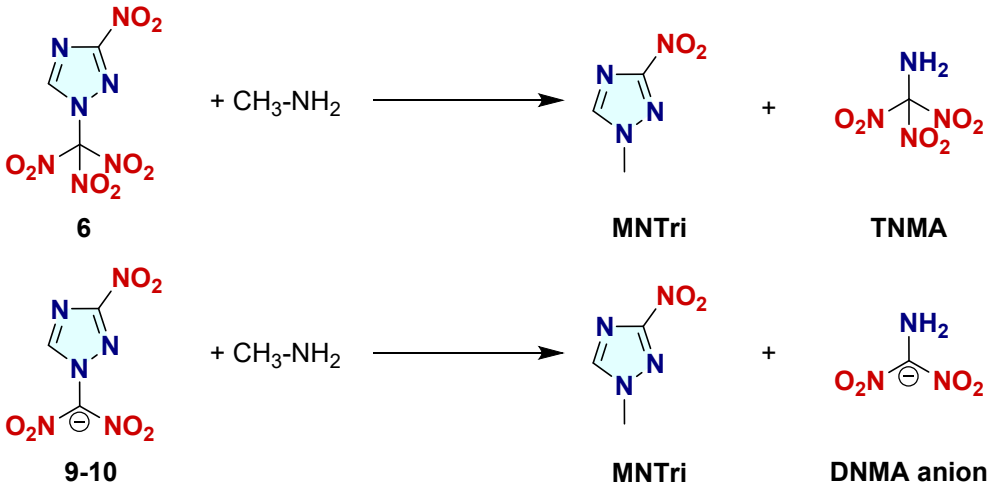



**Fig. S1**: Isodesmic reactions for compounds **6** and **9-10**.

For compound **5**, the solid-phase enthalpy of formation $\Delta H_f°$ (s) was calculated by using equation 1.[2-3]

$$\Delta H_f°(s) = \Delta H_f°(g) - \Delta H_{sub} \quad (1)$$

Where, $\Delta H_f°(s)$ is the solid phase enthalpy of formation, $\Delta H_f°(g)$ is gas phase enthalpy of formation and $\Delta H_{sub}$ is the enthalpy of sublimation.

The enthalpy of sublimation was estimated using equation 2 based on Trouton's rule:[3,4]

$$\Delta H_{sub} = 0.188 \times T/kJmol^{-1}K^{-1} \quad (2)$$

where, *T*, is either the melting point (mp) or the decomposition temperature ($T_d$), when melting does not occur before decomposition.

For salts **9-10**, the solid phase enthalpies of formation were obtained using the Born-Haber energy cycle.[3]

The bond dissociation energies (BDEs) of compound **6** were estimated according to equation 3.

$$BDE\ [AB] = E_0\ [A.] + E_0\ [B.] - E_0\ [AB] \quad (3)$$

where, BDE [AB] is bond dissociation energy and $E_0$ [A.] and $E_0$ [B.] are the energies of the individual homolytic part and $E_0$ [AB] is the total energy of the individual molecule.

**Table S2.** The standard enthalpies of combustion, $\Delta H_f^\circ{}_{(combust)}$, for the title compounds were calculated by equations 4-8.

$$\Delta H_f^\circ{}_{(combust)} = \Sigma \Delta H_f^\circ{}_{(products)} - \Sigma \Delta H_f^\circ{}_{(reactants)} \quad (4)$$

**RDX** = $C_3H_6N_6O_6$ (s) + 1.5 $O_2$ (g) $\longrightarrow$ 3$CO_2$ (g) + 3$H_2O$ (g) + 3$N_2$ (g) (5)

**HMX** = $C_4H_8N_8O_8$ (s) + 2.0 $O_2$ (g) $\longrightarrow$ 4$CO_2$ (g) + 4$H_2O$ (g) + 4$N_2$ (g) (6)

**6** = $C_3HN_7O_8$ (s) $\longrightarrow$ 3$CO_2$ (g) + 0.5$H_2O$ (g) + 3.5$N_2$ (g) + 0.75 $O_2$ (g) (7)

**9** = $C_3H_6N_8O_6$ (s) + 1.5 $O_2$ (g) $\longrightarrow$ 3$CO_2$ (g) + 3$H_2O$ (g) + 4$N_2$ (g) (8)

The standard enthalpy of formation for $CO_2$ ($\Delta H_f^\circ{}_{(CO2)}$ = -393.51 kJmol$^{-1}$); $H_2O$ ($\Delta H_f^\circ{}_{(H2O)}$ = -243.015 kJmol$^{-1}$).

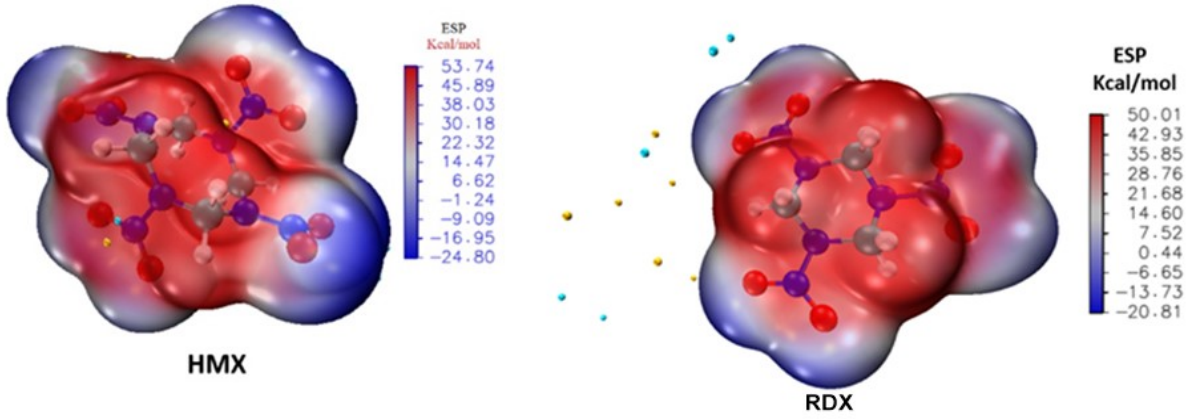



**Fig. S2:** Computed electrostatic potential (ESP) maps of RDX and HMX.

**Table S3**. Comparison of the ratio of positive and negative ESPs and the surface area of ESPs of compounds and positive variance, total variance, balance of charges and product of total variance and balance of charges.

| Compounds | $A_{tot}$[a] Å$^2$ | $A_{pos}$[b] Å$^2$ | $A_{neg}$[c] Å$^2$ | $ratio_{pos}$ (%) | $ratio_{neg}$ (%) | $\sigma^2_{tot}\upsilon$[d] (kcal/mol) |
|---|---|---|---|---|---|---|
| **6** | 223.13 | 133.50 | 89.63 | 59.83 | 40.17 | 44.62 |
| **9** | 253.42 | 98.34 | 155.08 | 38.80 | 61.20 | 135.33 |
| **RDX** | 209.49 | 116.77 | 92.72 | 55.74 | 44.26 | 27.29 |
| **HMX** | 251.50 | 131.14 | 120.36 | 52.14 | 47.86 | 33.09 |

[a]$SA_{tot}$ = Total surface area. [b]$SA_{pos}$ = positive surface area. [c]$SA_{neg}$ = Negative surface area. [d]Ratio of positive surface area [e] [d]Ratio of negative surface area. [g]Product of total variance and balance of charges.

## EXPERIMENTAL SECTION

### General Methods

All reagents and solvents were used as received unless otherwise specified (AKSci, Sigma-Aldrich, Acros Organics, VWR). The densities of the new compounds were obtained at 25 °C with a Micromeritics Accupyc II 1340 gas pycnometer. The thermal stability (melting and decomposition points) was measured by heating individual samples from 35 °C to 400 °C at the heating rate of 5 °C and 10 °C min$^{-1}$ on a Differential Scanning Calorimeter (DSC, TA Instruments Company, Model: Q2000) and thermogravimetric analysis (TGA, TA Instruments Company, Model: Q50). The FTIR spectra were recorded with KBr plates on a Thermo Nicolet AVATAR 370

spectrometer. $^{1}H$ and $^{13}C$ NMR spectra were recorded on a 500 MHz (Brucker) nuclear magnetic resonance spectrometer operating at 500.19 and 125.77 MHz, respectively, using DMSO-$d_6$ as the solvent and locking solvent. The $^{15}N$ NMR spectra were recorded on a 500.19 MHz (Brucker 500) nuclear magnetic resonance operating at 50.70 MHz. As external standards, the chemical shifts are given relative to tetramethylsilane ($^{1}H$, $^{13}C$) and nitromethane ($^{15}N$). Elemental analyses (C, H, N) were performed using a Vario Micro cube Elemental Analyser. The friction sensitivities (FS) and impact sensitivities (IS) were measured with a standard BAM friction tester and BAM drop hammer.[9] Crystals of **6** and **9** was mounted on a nylon loop with Paratone oil on an XtaLAB Synergy, Dualflex, HyPix diffractometer at 100 K. The structures were solved with the ShelXT[5-7] solution program using dual methods and Olex2.[8] The model was refined with ShelXL34 using full matrix least squares minimization on $F^2$.

***Caution!***

The compounds studied in the present work are potentially high-energy materials. Therefore, it is strongly recommended that these compounds should be synthesized and handled with extreme care and follow all the standard safety precautions.

***3-Nitro-1-(trinitromethyl)-1H-1,2,4-triazole*** **(6).** $H_2SO_4$ (98%, 6.4 mL, 120 mmol, 10.0 equiv.) was cooled at 0 °C, and fuming $HNO_3$ (5.04 mL, 120 mmol, 10.0 equiv.) was added to this dropwise, and the resulting mixture was stirred for 15 min at the same temperature. Compound **8** (2.01 g, 12 mmol, 1.0 equiv.) was added portion-wise. The resulting reaction mixture was stirred at room temperature for 36 h and poured into ice-cold water. The white solid was filtered off, dried, and recrystallized with methanol. Crystalline, white solid; Yield: 2.28 g, 72%, DSC (5 °C $min^{-1}$): $T_m$ = 101 °C (melting

point). $T_{d\ (onset)}$ 138 °C; IR (KBr pellet) υ 3151 (s), 2885 (m), 1616 (s), 1571 (s), 1524 (s), 1440 (m), 1378 (s), 1348 (m), 1301 (s), 1276 (s), 1237 (s), 1057 (m), 942 (m), 877 (m), 837 (s), 798 (s), 641 (s) $cm^{-1}$; $^{1}H$ NMR (500.19 MHz, DMSO-$d_6$): d 9.79 (s, 1H); $^{13}C$ NMR (125.77 MHz, DMSO-$d_6$): d 164.4, 152.9, 118.3; $^{13}C$ NMR (125.77 MHz, DMSO-$d_6$): d -33.21, -39.89, -90.09, -127.03, -183.71; Elemental analysis: calcd (%) for $C_3HN_7O_8$ (263.08): C, 13.70; H, 0.38; N, 37.27. Found C, 13.74; H, 0.63; N, 36.89.

***1-(3-Nitro-1H-1,2,4-triazol-1-yl)propan-2-one*** **(8).** Commercially available 3-nitro-1*H*-1,2,4-triazole **7** (2.850 g, 25 mmol, 1.0 equiv.) was dissolved in water (10 mL), and NaOH (1.100 g, 55 mmol, 1.1 equiv.) was added at below 10 °C. The resulting reaction mixture was stirred at below 10 °C for one hour, a solution of chloroacetone (2.550 g, 27.5 mmol, 1.1 equiv.) in acetone (10 mL) was added, and the resulting reaction mixture was stirred at room temperature overnight. The solvent (acetone) was evaporated, residue was diluted with water (20 mL), and filtered to give a crude compound, which was further purified by recrystallization with acetonitrile. Crystalline, light-yellow solid; Yield: 4.04 g, 95%, DSC (5 °C $min^{-1}$): $T_m$ = 101°C (melting point). $T_{d\ (onset)}$ 227 °C; IR (KBr pellet) υ 3454 (m), 3107 (s), 2989 (m), 2951 (m), 1735 (s), 1555 (s), 1503 (s), 1413 (s), 1373 (s), 1342 (S), 1308 (s), 1215 (s), 1179 (s), 1042 (m), 902 (m), 840 (s), 781 (m), 658 (m) $cm^{-1}$; $^{1}H$ NMR (500.19 MHz, DMSO-$d_6$): d 8.73 (s, 1H), 5.50 (s, 2H), 2.25 (s, 3H); $^{13}C$ NMR (125.77 MHz, DMSO-$d_6$): d 200.0, 162.0, 148.0, 59.2, 27.0; Elemental analysis: calcd (%) for $C_5H_6N_4O_3$ (170.13): C, 31.85; H, 2.67; N, 29.71. Found C, 32.26; H, 2.84; N, 28.96.

***Hydrazinium dinitro(3-nitro-1H-1,2,4-triazol-1-yl)methanide*** **(9).** Compound **6** (1.05 g, 4.0 mmol, 1.0 equiv.) was dissolved in methanol, and hydrazine hydrate (0.4 g, 8.0

mmol, 2.0 equiv.) was added dropwise; a red ppt formed, and the suspension was stirred for 6 h at 0°C. The solvent was evaporated, and the solid taken up in acetonitrile and the reaction mixture was filtered to give a crude compound, which was further purified by recrystallization with methanol. Crystalline, red brown solid; Yield: 0.96 g, 96%, DSC (5 °C $min^{-1}$): $T_{d\ (onset)}$ 137 °C; IR (KBr pellet) υ 3348 (s), 3195 (s), 2966 (s), 2774 (m), 2631 (m), 1565 (s), 1498 (s), 1423 (s), 1395 (s), 1310 (s), 1255 (s), 1214 (s), 1111 (s), 1014 (m), 980 (s), 907 (m), 838 (m), 826 (m), 792 (w), 768 (w), 748 (m), 739 (s), 721 (m), 657 (w), 618 (s) $cm^{-1}$; $^{1}H$ NMR (500.19 MHz, DMSO-$d_6$): d 9.13 (s, 1H), 7.02 (br s, 5H); $^{13}C$ NMR (125.77 MHz, DMSO-$d_6$): d 162.8, 151.9, 130.5; Elemental analysis: calcd (%) for $C_3H_6N_8O_6$ (250.13): C, 14.41; H, 2.42; N, 44.80. Found C, 14.42; H, 2.08; N, 44.54.

***Potassium dinitro(3-nitro-1H-1,2,4-triazol-1-yl)methanide*** **(10.$H_2O$).** Compound **6** (1.05 g, 4.0 mmol, 1.0 equiv.) was dissolved in methanol (5 mL), and KI (1.33 g, 8.0 mmol, 2.0 equiv.) was added portion-wise; a red brown ppt formed, and further stirred overnight at 25 °C. The solvent was evaporated, and acetonitrile (10 mL) added to give a crude mixture which was filtered. The solid was taken up in methanol and further purified by recrystallization with methanol. Crystalline, red brown solid; Yield: 1.08 g, 98%, DSC (5 °C $min^{-1}$): $T_{d\ (onset)}$ 225 °C; IR (KBr pellet) υ 3440 (m), 3110 (s), 1565 (s), 1530 (s), 1493 (s), 1422 (s), 1382 (s), 1353 (m), 1309 (s), 1219 (s), 1154 (s), 1072 (w), 982 (m), 840 (m), 740 (m) $cm^{-1}$; $^{1}H$ NMR (500.19 MHz, DMSO-$d_6$): d 9.14 (s, 1H); $^{13}C$ NMR (125.77 MHz, DMSO-$d_6$): d 162.7, 151.9, 130.4; Elemental analysis: calcd (%) for $C_3HKN_6O_6.H_2O$ (274.19): C, 13.14; H, 1.10; N, 30.65. Found C, 13.49; H, 0.578; N, 30.84.

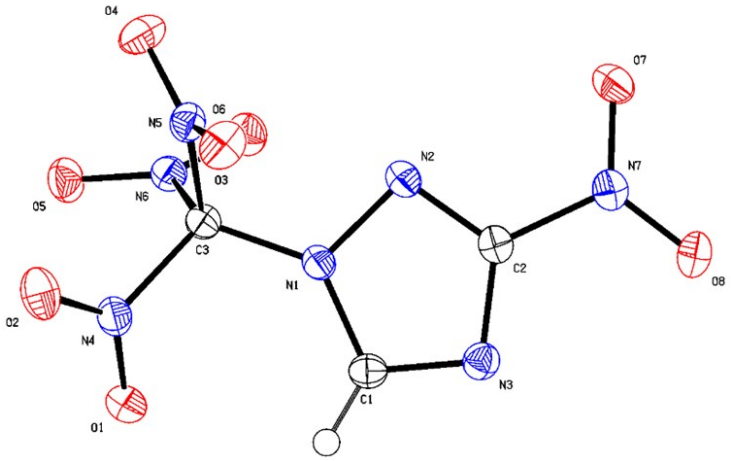



**Fig. S3**: Single crystal X-ray structure of compound **6**.

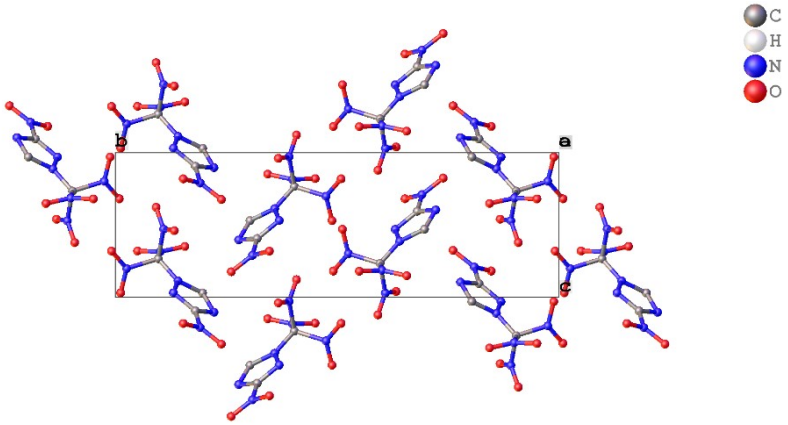



**Fig. S4**: Packing diagram of compound **6**.

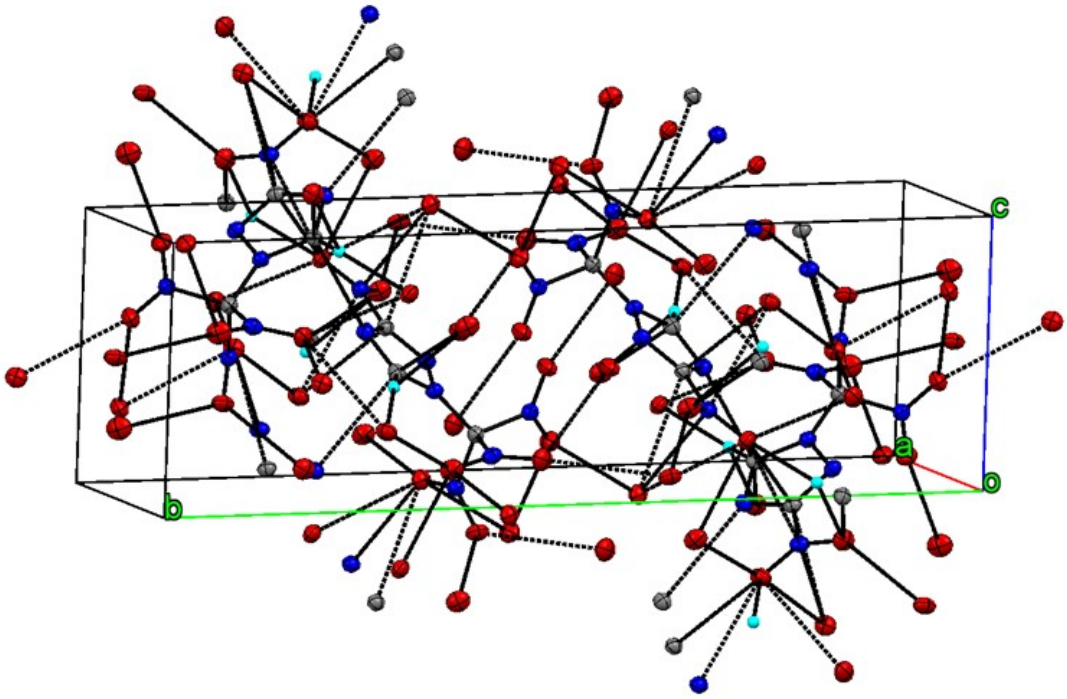
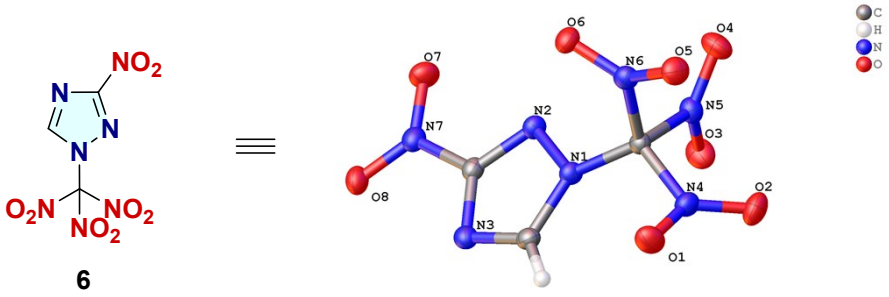



**Fig. S5**: Packing diagram of compound **6**.

**Table S4**. Single crystal X-ray data and structure refinement for compound **6**.[5-8]



| Compound | 6 |
|---|---|
| CCDC | 2253474 |
| Formula | $C_3HN_7O_8$ |
| $D_{calc.}$/ g cm$^{-3}$ | 1.999 |
| $m$/mm$^{-1}$ | 1.790 |
| Formula Weight | 263.11 |
| Color | colorless |
| Shape | needle-shaped |
| Size/mm$^3$ | 0.24×0.04×0.02 |
| $T$/K | 100.0(3) |
| Crystal System | monoclinic |
| Space Group | $P2_1/c$ |
| $a$/Å | 6.5694(2) |
| $b$/Å | 20.2409(5) |
| $c$/Å | 6.5938(2) |
| $a$/° | 90 |
| $b$/° | 94.206(2) |
| $g$/° | 90 |
| V/Å$^3$ | 874.42(4) |
| $Z$ | 4 |
| $Z'$ | 1 |
| Wavelength/Å | 1.54184 |
| Radiation type | Cu $K_a$ |
| $Q_{min}$/° | 4.369 |
| $Q_{max}$/° | 80.468 |
| Measured Refl's. | 7932 |
| Indep't Refl's | 7932 |
| Refl's I≥2 $s$(I) | 7045 |
| $R_{int}$ | . |
| Parameters | 164 |
| Restraints | 0 |
| Largest Peak | 0.377 |
| Deepest Hole | -0.309 |
| GooF | 1.069 |
| $wR_2$ (all data) | 0.1071 |
| $wR_2$ | 0.1036 |
| $R_1$ (all data) | 0.0430 |
| $R_1$ | 0.0382 |

**Table S5**: Bond Angles in ° for compound **6**.

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| $N^2$ | $N^1$ | $C^1$ | 110.15(14) |
| $N^2$ | $N^1$ | $C^3$ | 115.88(13) |
| $C^1$ | $N^1$ | $C^3$ | 133.86(14) |
| $C^2$ | $N^2$ | $N^1$ | 100.16(13) |
| $C^1$ | $N^3$ | $C^2$ | 102.09(14) |
| O1 | N4 | C3 | 113.97(14) |
| O2 | N4 | O1 | 128.83(16) |
| O2 | N4 | C3 | 117.11(15) |
| O3 | N5 | O4 | 129.42(15) |

| Atom | Atom | Atom | Angle/° |
|---|---|---|---|
| O3 | N5 | C3 | 114.13(14) |
| O4 | N5 | C3 | 116.45(14) |
| O5 | N6 | C3 | 115.37(14) |
| O6 | N6 | O5 | 128.57(16) |
| O6 | N6 | C3 | 116.05(14) |
| O7 | N7 | C2 | 117.27(15) |
| O8 | N7 | O7 | 125.60(14) |
| O8 | N7 | C2 | 117.11(14) |
| N3 | C1 | N1 | 109.42(14) |
| N2 | C2 | N3 | 118.18(15) |
| N2 | C2 | N7 | 119.33(15) |
| N3 | C2 | N7 | 122.42(16) |
| N1 | C3 | N4 | 112.59(14) |
| N1 | C3 | N5 | 109.50(14) |
| N1 | C3 | N6 | 113.18(13) |
| N4 | C3 | N5 | 108.26(12) |
| N4 | C3 | N6 | 105.49(13) |
| N5 | C3 | N6 | 107.56(13) |

**Table S6**: Bond Lengths in Å for compound **6**.

| Atom | Atom | Length/Å |
|---|---|---|
| $O^1$ | $N^4$ | 1.216(2) |
| $O^2$ | $N^4$ | 1.206(2) |
| $O^3$ | $N^5$ | 1.208(2) |
| $O^4$ | $N^5$ | 1.209(2) |
| $O^5$ | $N^6$ | 1.216(2) |
| $O^6$ | $N^6$ | 1.208(2) |
| $O^7$ | $N^7$ | 1.222(2) |
| $O^8$ | $N^7$ | 1.222(2) |
| $N^1$ | $N^2$ | 1.368(2) |
| N1 | C1 | 1.372(2) |
| N1 | C3 | 1.410(2) |
| N2 | C2 | 1.300(2) |
| N3 | C1 | 1.307(2) |
| N3 | C2 | 1.355(2) |
| N4 | C3 | 1.526(2) |
| N5 | C3 | 1.543(2) |
| N6 | C3 | 1.548(2) |
| N7 | C2 | 1.459(2) |

**Table S7**: Torsion Angles in ° for compound **6.**

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| $O^1$ | $N^4$ | $C^3$ | $N^1$ | -52.2(2) |
| $O^1$ | $N^4$ | $C^3$ | $N^5$ | -173.43(15) |
| $O^1$ | $N^4$ | $C^3$ | $N^6$ | 71.66(17) |
| $O^2$ | $N^4$ | $C^3$ | $N^1$ | 130.99(17) |
| $O^2$ | $N^4$ | $C^3$ | $N^5$ | 9.8(2) |
| $O^2$ | $N^4$ | $C^3$ | $N^6$ | -105.12(17) |
| $O^3$ | $N^5$ | $C^3$ | $N^1$ | -49.74(18) |

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| $O^3$ | $N^5$ | $C^3$ | $N^4$ | 73.36(17) |
| $O^3$ | $N^5$ | $C^3$ | $N^6$ | -173.11(13) |
| $O^4$ | $N^5$ | $C^3$ | $N^1$ | 130.71(15) |
| $O^4$ | $N^5$ | $C^3$ | $N^4$ | -106.19(16) |
| $O^4$ | $N^5$ | $C^3$ | $N^6$ | 7.35(19) |
| $O^5$ | $N^6$ | $C^3$ | $N^1$ | 152.27(14) |
| $O^5$ | $N^6$ | $C^3$ | $N^4$ | 28.75(17) |
| $O^5$ | $N^6$ | $C^3$ | $N^5$ | -86.64(16) |
| $O^6$ | $N^6$ | $C^3$ | $N^1$ | -28.2(2) |
| $O^6$ | $N^6$ | $C^3$ | $N^4$ | -151.68(14) |
| $O^6$ | $N^6$ | $C^3$ | $N^5$ | 92.93(16) |
| $O^7$ | $N^7$ | $C^2$ | $N^2$ | -0.9(2) |
| $O^7$ | $N^7$ | $C^2$ | $N^3$ | 175.82(16) |
| $O^8$ | $N^7$ | $C^2$ | $N^2$ | -179.34(16) |
| $O^8$ | $N^7$ | $C^2$ | $N^3$ | -2.6(2) |
| $N^1$ | $N^2$ | $C^2$ | $N^3$ | -0.2(2) |
| $N^1$ | $N^2$ | $C^2$ | $N^7$ | 176.71(14) |
| $N^2$ | $N^1$ | $C^1$ | $N^3$ | 0.8(2) |
| $N^2$ | $N^1$ | $C^3$ | $N^4$ | -166.59(14) |
| $N^2$ | $N^1$ | $C^3$ | $N^5$ | -46.09(19) |
| $N^2$ | $N^1$ | $C^3$ | $N^6$ | 73.89(18) |
| $C^1$ | $N^1$ | $N^2$ | $C^2$ | -0.35(18) |
| $C^1$ | $N^1$ | $C^3$ | $N^4$ | 17.5(3) |
| $C^1$ | $N^1$ | $C^3$ | $N^5$ | 138.04(18) |
| $C^1$ | $N^1$ | $C^3$ | $N^6$ | -102.0(2) |
| $C^1$ | $N^3$ | $C^2$ | $N^2$ | 0.6(2) |
| $C^1$ | $N^3$ | $C^2$ | $N^7$ | -176.15(16) |
| $C^2$ | $N^3$ | $C^1$ | $N^1$ | -0.80(19) |
| $C^3$ | $N^1$ | $N^2$ | $C^2$ | -177.18(15) |
| $C^3$ | $N^1$ | $C^1$ | $N^3$ | 176.82(18) |

**Table S8**: Hydrogen Fractional Atomic Coordinates (×$10^4$) and Equivalent Isotropic Displacement Parameters (Å$^2$×$10^3$) for compound **6**. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$.

| Atom | x | Y | z | $U_{eq}$ |
|---|---|---|---|---|
| $H^1$ | 9024.52 | 2860.99 | 5644.72 | 22 |

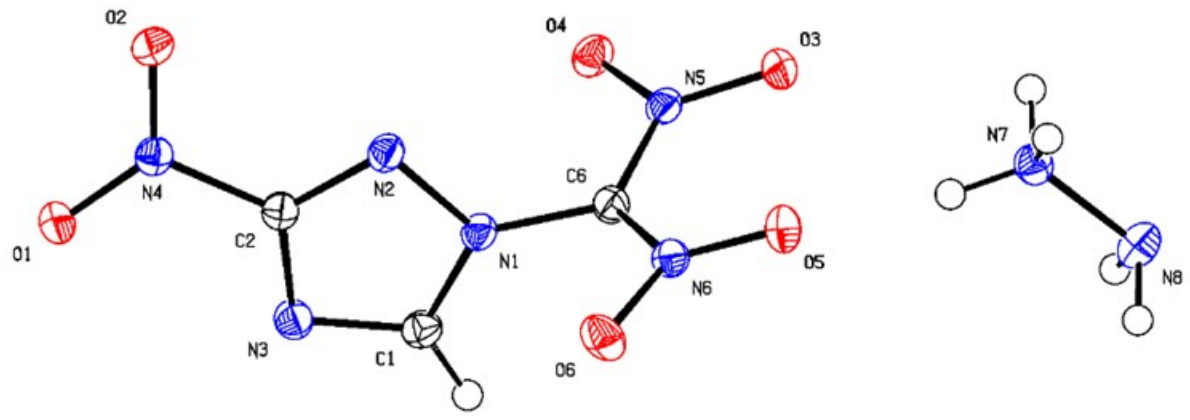


**Fig. S6**: Single crystal X-ray structure of compound **9**.

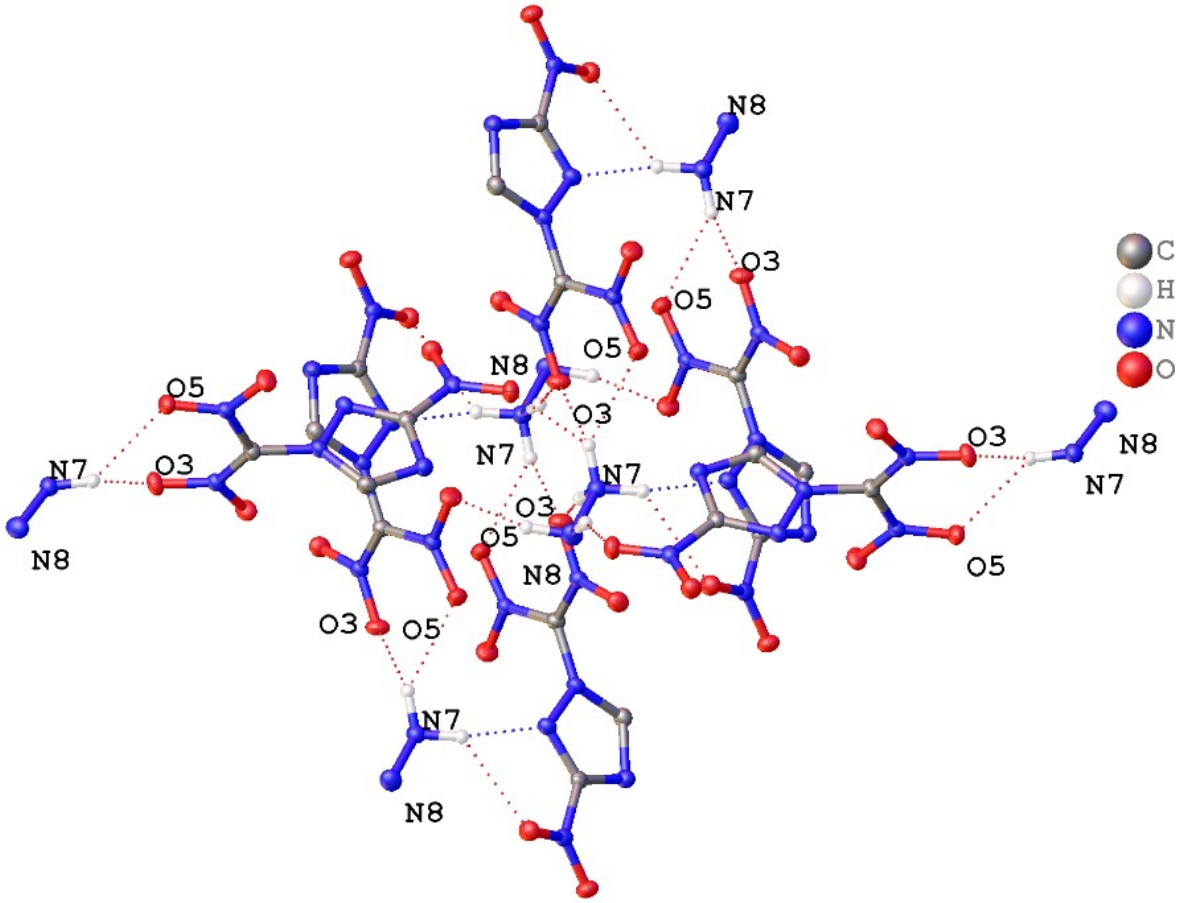



**Fig. S7**: The following hydrogen bonding interactions with a maximum D-D distance of 3.1 Å and a minimum angle of 110 ° are present in compound **9**: N7–O1_*1: 2.994 Å, N7–O2*_2: 3.075 Å, N7–O3: 2.878 Å, N7–O3_*3: 2.927 Å, N7–O4*_3: 3.089 Å, N7–O5: 2.961 Å, N7–N2_*2: 3.009 Å, N8–O1*_4: 3.056 Å, N8–O6_*5: 3.002 Å.*

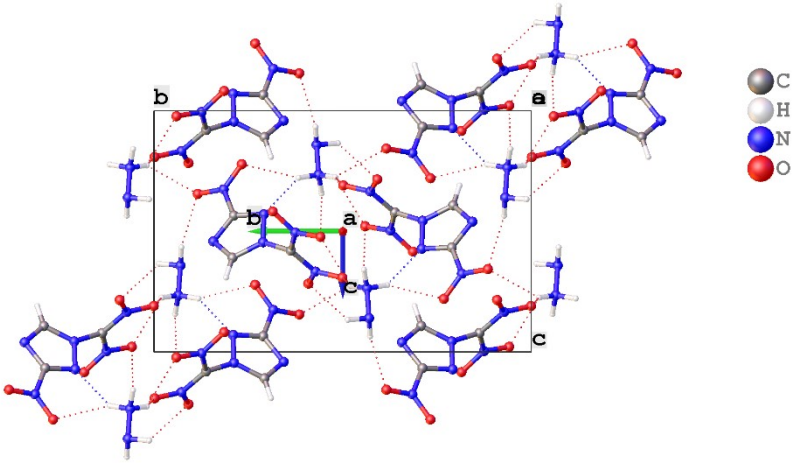



**Fig. S8**: Packing diagram of compound **9** viewed along the **a** axis

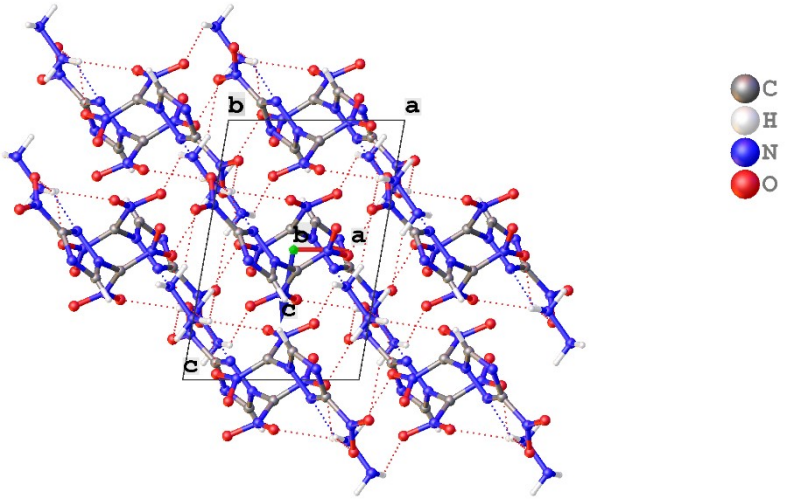



**Fig. S9**: Packing diagram of compound **9** viewed along the **b** axis

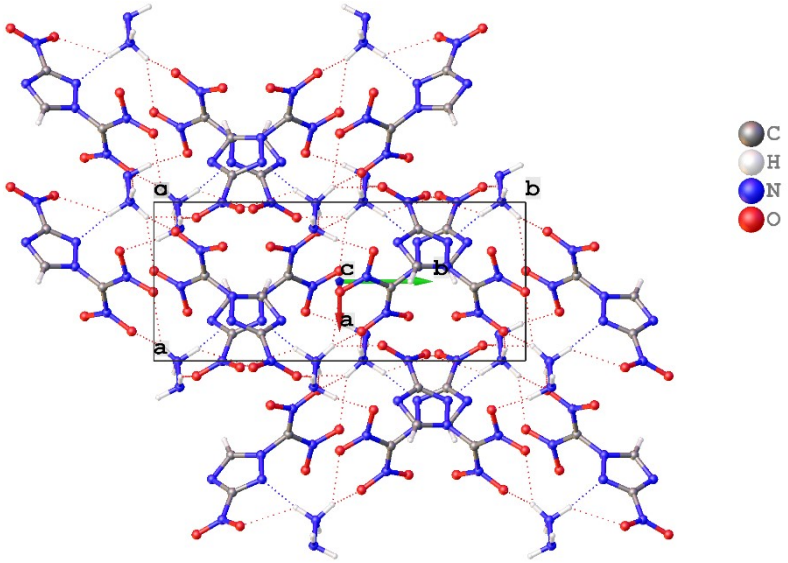
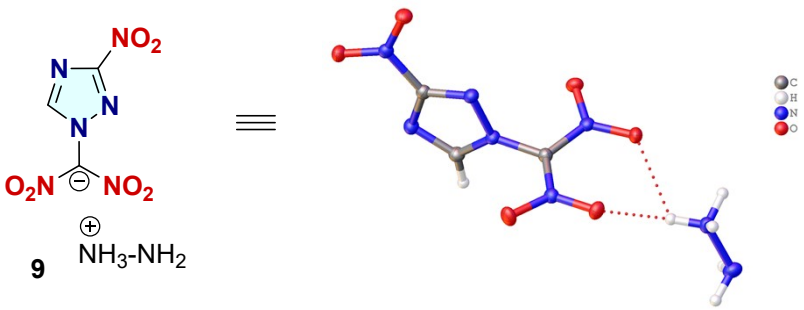



**Fig. S10**: Packing diagram of compound **9** viewed along the **c** axis

**Table S9**. Single crystal X-ray data and structure refinement for compound **9**.[5-8]



| Compound | 9 |
|---|---|
| CCDC | 2255083 |
| Formula | $C_3H_6N_8O_6$ |
| $D_{calc.}$/ g cm$^{-3}$ | 1.809 |
| $m$/mm$^{-1}$ | 1.516 |
| Formula Weight | 250.16 |
| Color | yellow |
| Shape | block-shaped |
| Size/mm$^3$ | 0.12×0.08×0.04 |
| $T$/K | 99.9(3) |
| Crystal System | monoclinic |
| Space Group | $P2_1/c$ |
| $a$/Å | 6.46056(13) |
| $b$/Å | 14.9402(3) |
| $c$/Å | 9.66552(18) |
| $a$/° | 90 |
| $b$/° | 100.0185(19) |
| $g$/° | 90 |
| V/Å$^3$ | 918.71(3) |
| $Z$ | 4 |
| $Z'$ | 1 |
| Wavelength/Å | 1.54184 |
| Radiation type | Cu $K_a$ |
| $Q_{min}$/° | 5.511 |
| $Q_{max}$/° | 80.244 |
| Measured Refl's. | 6794 |
| Indep't Refl's | 1949 |
| Refl's I≥2 $s$(I) | 1760 |
| $R_{int}$ | 0.0324 |
| Parameters | 174 |
| Restraints | 0 |
| Largest Peak | 0.274 |
| Deepest Hole | -0.299 |
| GooF | 1.099 |
| $wR_2$ (all data) | 0.0920 |
| $wR_2$ | 0.0895 |
| $R_1$ (all data) | 0.0371 |
| $R_1$ | 0.0336 |

**Table S10**: Bond Lengths in Å for compound **9**.

| Atom | Atom | Length/Å |
|---|---|---|
| $O^1$ | $N^4$ | 1.2272(15) |
| $O^2$ | $N^4$ | 1.2237(15) |
| $O^3$ | $N^5$ | 1.2513(15) |
| $O^4$ | $N^5$ | 1.2471(15) |
| $O^5$ | $N^6$ | 1.2377(15) |
| $O^6$ | $N^6$ | 1.2526(15) |
| $N^1$ | $N^2$ | 1.3624(16) |
| $N^1$ | $C^1$ | 1.3524(18) |
| $N^1$ | $C^6$ | 1.3989(17) |
| $N^2$ | $C^2$ | 1.3067(17) |
| $N^3$ | $C^1$ | 1.3224(18) |

| Atom | Atom | Length/Å |
|---|---|---|
| $N^3$ | $C^2$ | 1.3480(17) |
| $N^4$ | $C^2$ | 1.4519(17) |
| $N^5$ | $C^6$ | 1.3785(17) |
| $N^6$ | $C^6$ | 1.3897(17) |
| $N^7$ | $N^8$ | 1.4412(17) |

**Table S11**: Torsion Angles in ° for compound **9**.

| Atom | Atom | Atom | Atom | Angle/° |
|---|---|---|---|---|
| $O^1$ | $N^4$ | $C^2$ | $N^2$ | -168.95(12) |
| $O^1$ | $N^4$ | $C^2$ | $N^3$ | 11.77(18) |
| $O^2$ | $N^4$ | $C^2$ | $N^2$ | 11.36(17) |
| $O^2$ | $N^4$ | $C^2$ | $N^3$ | -167.92(12) |
| $O^3$ | $N^5$ | $C^6$ | $N^1$ | 175.76(11) |
| $O^3$ | $N^5$ | $C^6$ | $N^6$ | 9.73(19) |
| $O^4$ | $N^5$ | $C^6$ | $N^1$ | -4.70(17) |
| $O^4$ | $N^5$ | $C^6$ | $N^6$ | -170.73(12) |
| $O^5$ | $N^6$ | $C^6$ | $N^1$ | -172.82(11) |
| $O^5$ | $N^6$ | $C^6$ | $N^5$ | -6.9(2) |
| $O^6$ | $N^6$ | $C^6$ | $N^1$ | 7.20(17) |
| $O^6$ | $N^6$ | $C^6$ | $N^5$ | 173.11(12) |
| $N^1$ | $N^2$ | $C^2$ | $N^3$ | 0.14(16) |
| $N^1$ | $N^2$ | $C^2$ | $N^4$ | -179.18(11) |
| $N^2$ | $N^1$ | $C^1$ | $N^3$ | -1.17(15) |
| $N^2$ | $N^1$ | $C^6$ | $N^5$ | -78.01(15) |
| $N^2$ | $N^1$ | $C^6$ | $N^6$ | 89.02(15) |
| $C^1$ | $N^1$ | $N^2$ | $C^2$ | 0.61(14) |
| $C^1$ | $N^1$ | $C^6$ | $N^5$ | 100.92(16) |
| $C^1$ | $N^1$ | $C^6$ | $N^6$ | -92.05(17) |
| $C^1$ | $N^3$ | $C^2$ | $N^2$ | -0.80(16) |
| $C^1$ | $N^3$ | $C^2$ | $N^4$ | 178.48(12) |
| $C^2$ | $N^3$ | $C^1$ | $N^1$ | 1.13(15) |
| $C^6$ | $N^1$ | $N^2$ | $C^2$ | 179.74(11) |
| $C^6$ | $N^1$ | $C^1$ | $N^3$ | 179.81(12) |

**Table S12**: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **9**. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{ij}$.

| Atom | x | y | z | $U_{eq}$ |
|---|---|---|---|---|
| $H^1$ | 5004.2 | 1904.46 | 3093.91 | 20 |
| $H^{7A}$ | 920(40) | 5199(16) | 2740(20) | 37(6) |
| $H^{7B}$ | 740(40) | 6173(17) | 2780(20) | 42(6) |
| $H^{7C}$ | -730(50) | 5558(18) | 3420(30) | 57(7) |
| $H^{8A}$ | -1020(40) | 5723(15) | 660(30) | 42(6) |
| $H^{8B}$ | -2320(40) | 5131(16) | 1340(20) | 42(6) |

**Table S13**: Hydrogen Bond information for compound **9**.

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/deg |
|---|---|---|---|---|---|---|
| $N^{7}$ | $H^{7A}$ | $O^{11}$ | 0.91(2) | 2.32(2) | 2.9945(16) | 130.7(17) |
| $N^{7}$ | $H^{7A}$ | $O^{3}$ | 0.91(2) | 2.29(2) | 2.8784(16) | 122.8(18) |
| $N^{7}$ | $H^{7A}$ | $O^{5}$ | 0.91(2) | 2.20(2) | 2.9607(16) | 141.2(19) |
| $N^{7}$ | $H^{7B}$ | $O^{22}$ | 0.94(3) | 2.40(2) | 3.0753(16) | 128.2(18) |
| $N^{7}$ | $H^{7B}$ | $N^{22}$ | 0.94(3) | 2.18(2) | 3.0088(16) | 146(2) |
| $N^{7}$ | $H^{7C}$ | $O^{33}$ | 0.94(3) | 2.00(3) | 2.9274(16) | 169(2) |
| $N^{7}$ | $H^{7C}$ | $O^{43}$ | 0.94(3) | 2.53(3) | 3.0887(16) | 118(2) |
| $N^{8}$ | $H^{8A}$ | $O^{14}$ | 0.89(3) | 2.24(3) | 3.0557(16) | 151(2) |
| $N^{8}$ | $H^{8B}$ | $O^{65}$ | 0.95(2) | 2.25(2) | 3.0021(16) | 136.4(19) |

[1]-1+x,1/2-y,-1/2+z; [2]1-x,1-y,1-z; [3]-x,1-y,1-z; [4]1-x,1/2+y,1/2-z; [5]-1+x,+y,+z

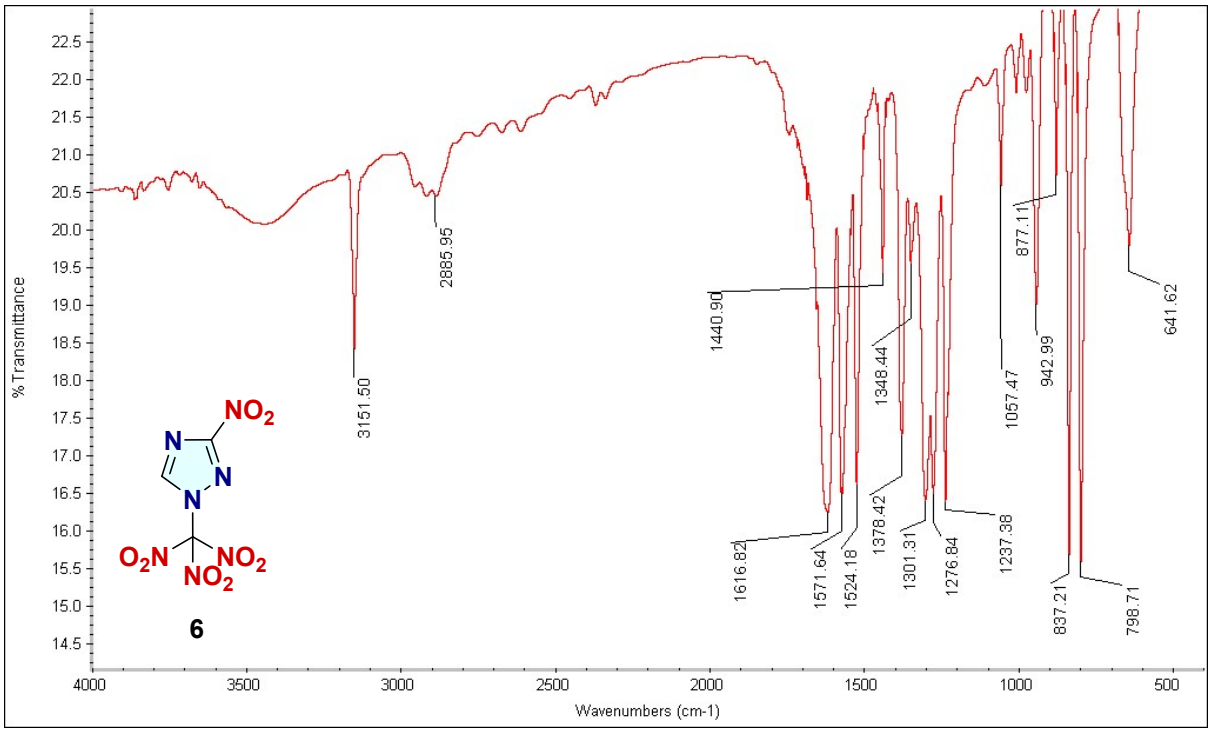



**Fig. S11:** FTIR-Spectrum of Compound **6**.

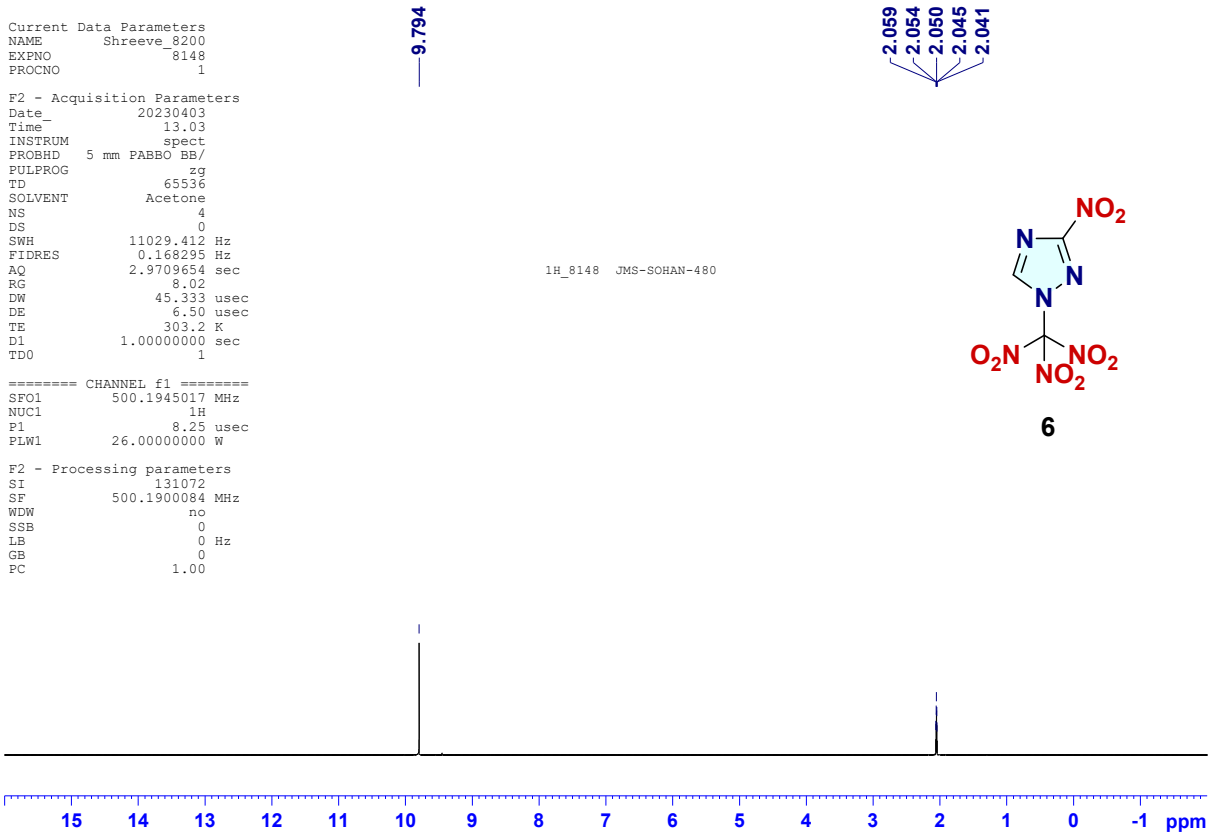



**Fig. S12**: $^{1}$H NMR Spectrum of Compound **6** (500.19 MHz).

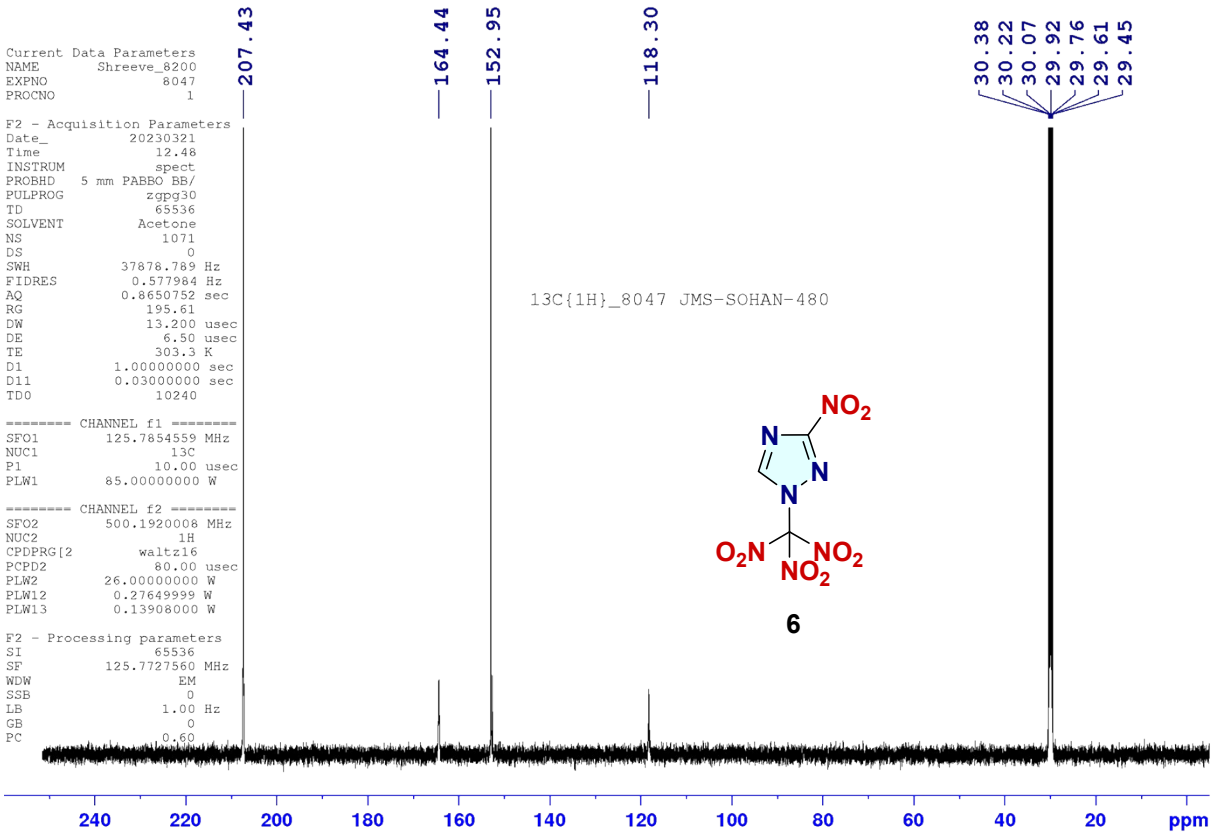



**Fig. S13**: $^{13}$C NMR Spectrum of Compound **6** (125.77 MHz).

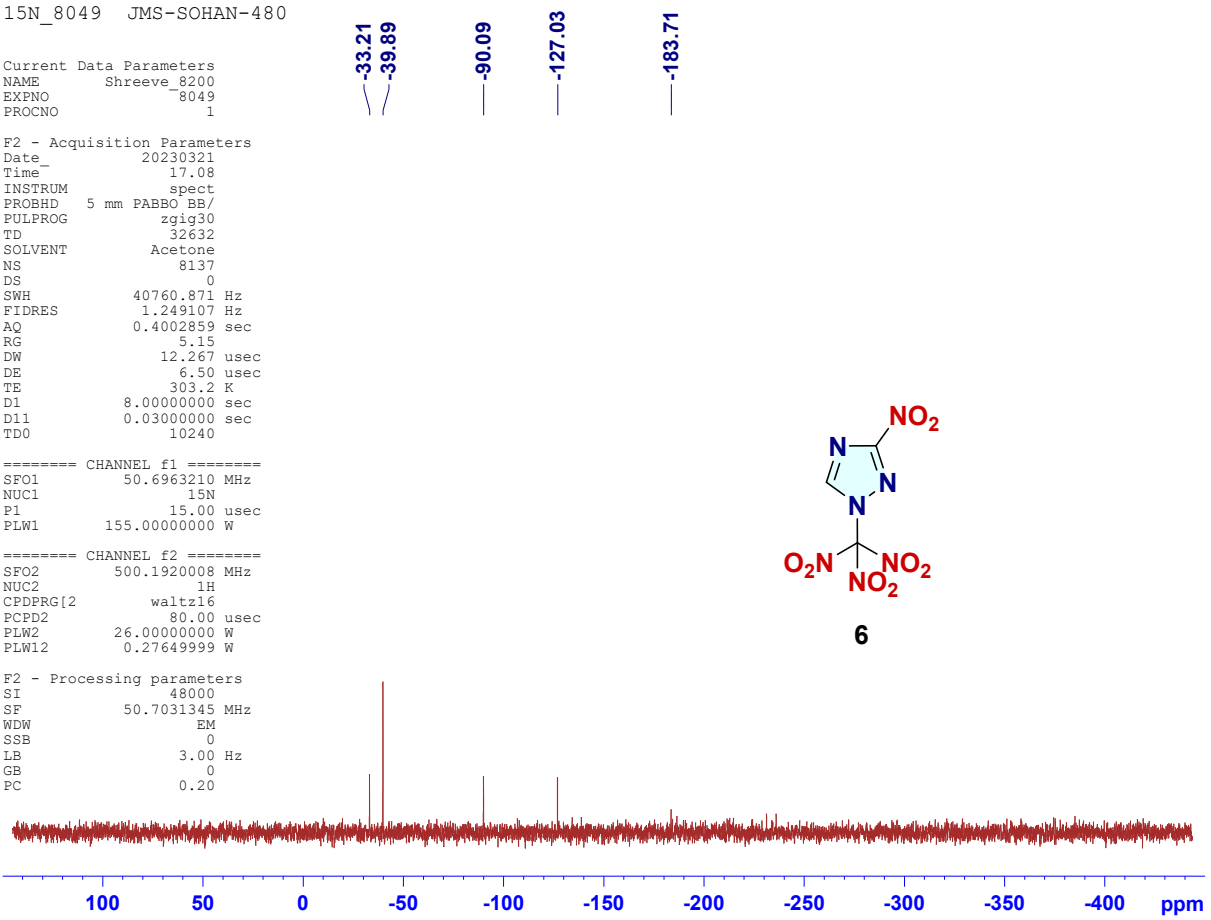



**Fig. S14**: $^{1}$H NMR Spectrum of Compound **6** (500.19 MHz).

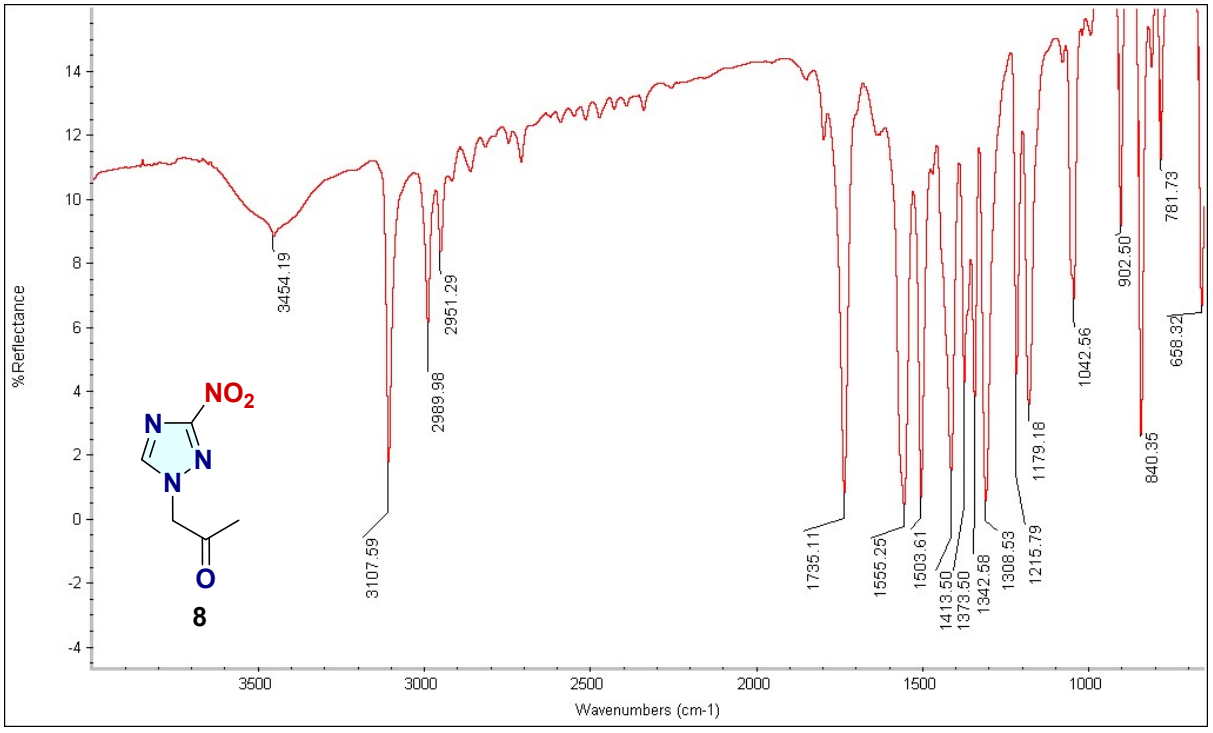



**Fig. S15:** FTIR-Spectrum of Compound **8**.

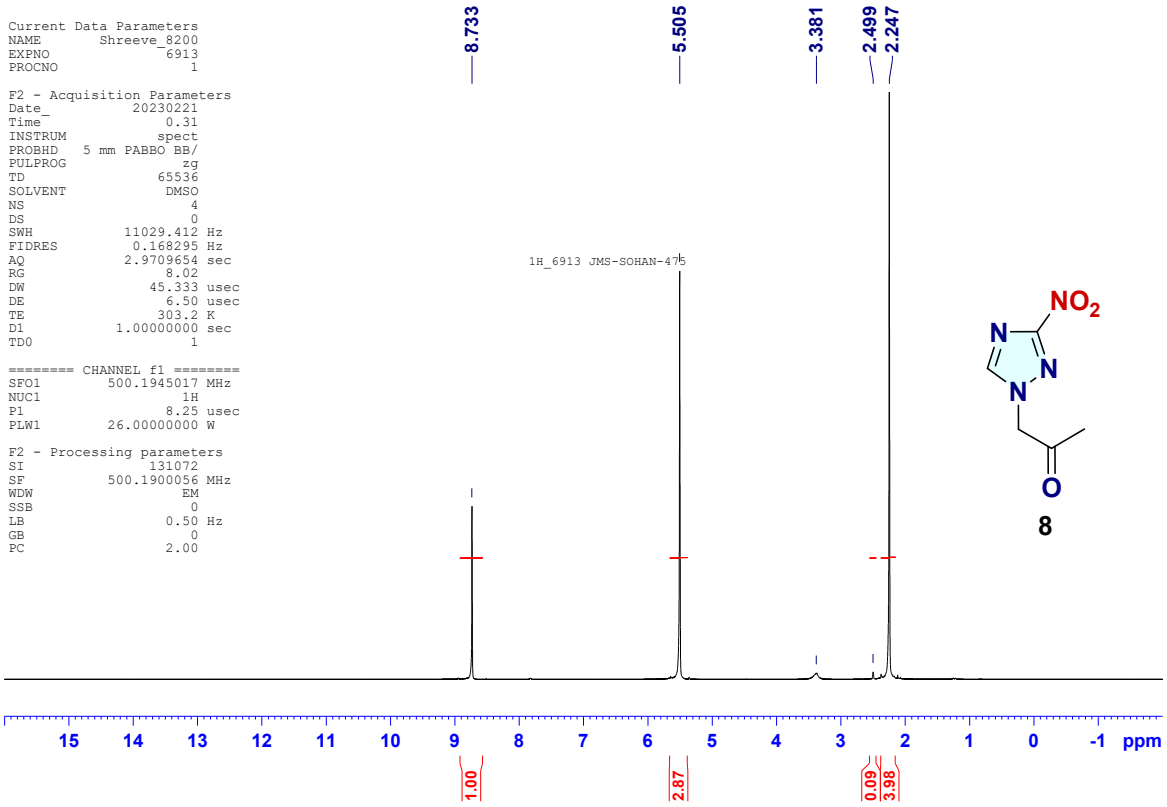



**Fig. S16**: $^{1}$H NMR Spectrum of Compound **8** (500.19 MHz).

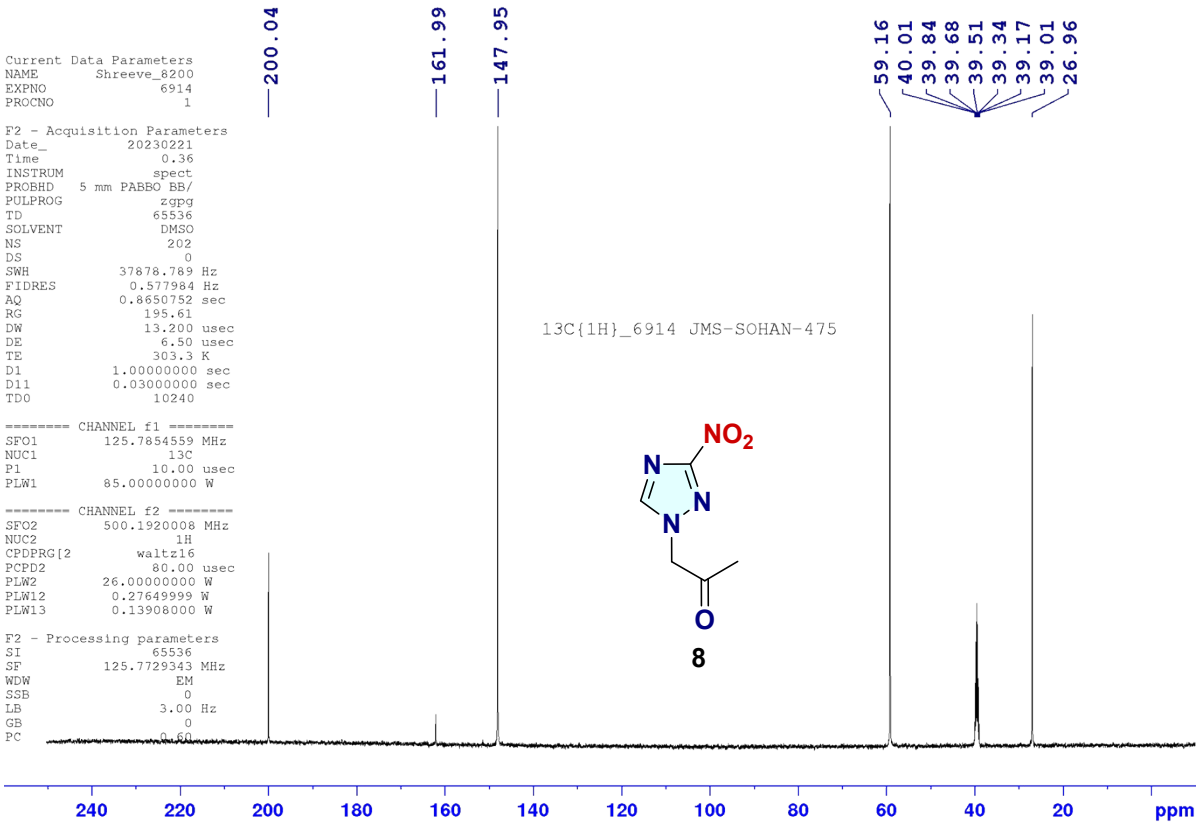



**Fig. S17**: $^{13}$C NMR Spectrum of Compound **8** (125.77 MHz).

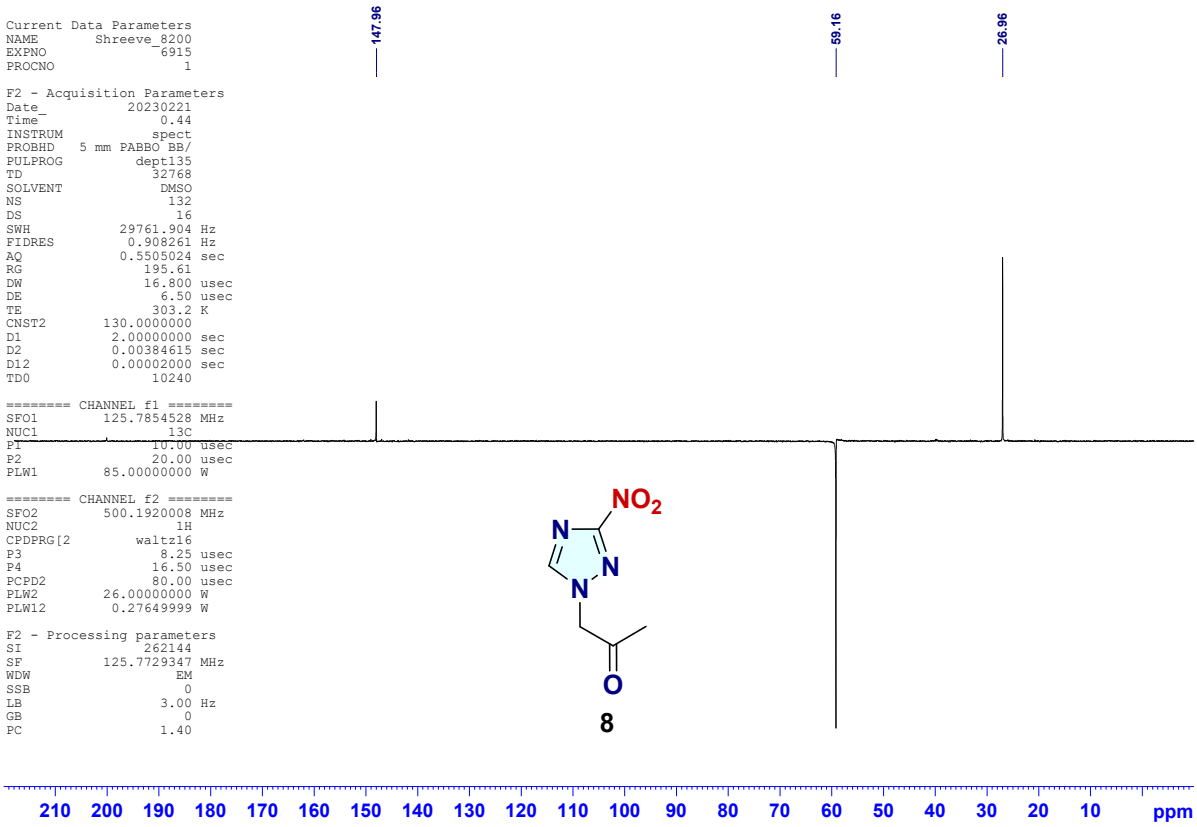



**Fig. S18**: $^{13}$C-DEPT NMR Spectrum of Compound **8** (125.77 MHz).

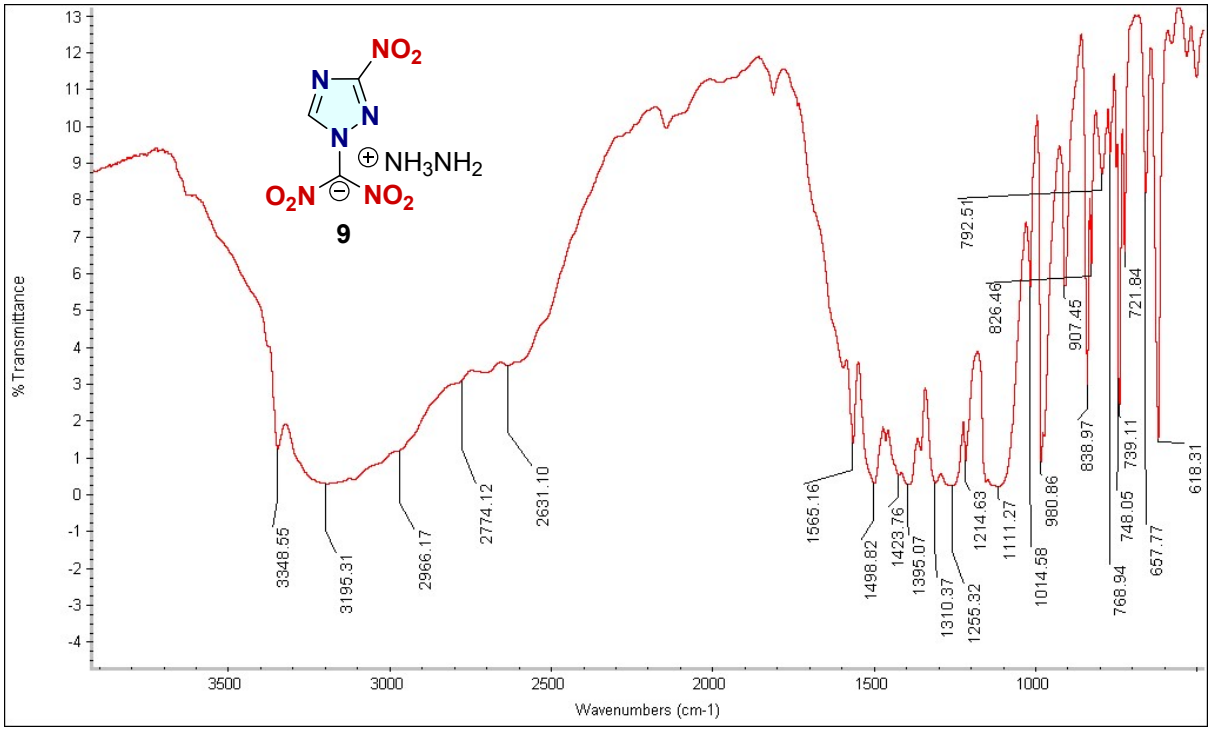



**Fig. S19:** FTIR-Spectrum of Compound **9**.

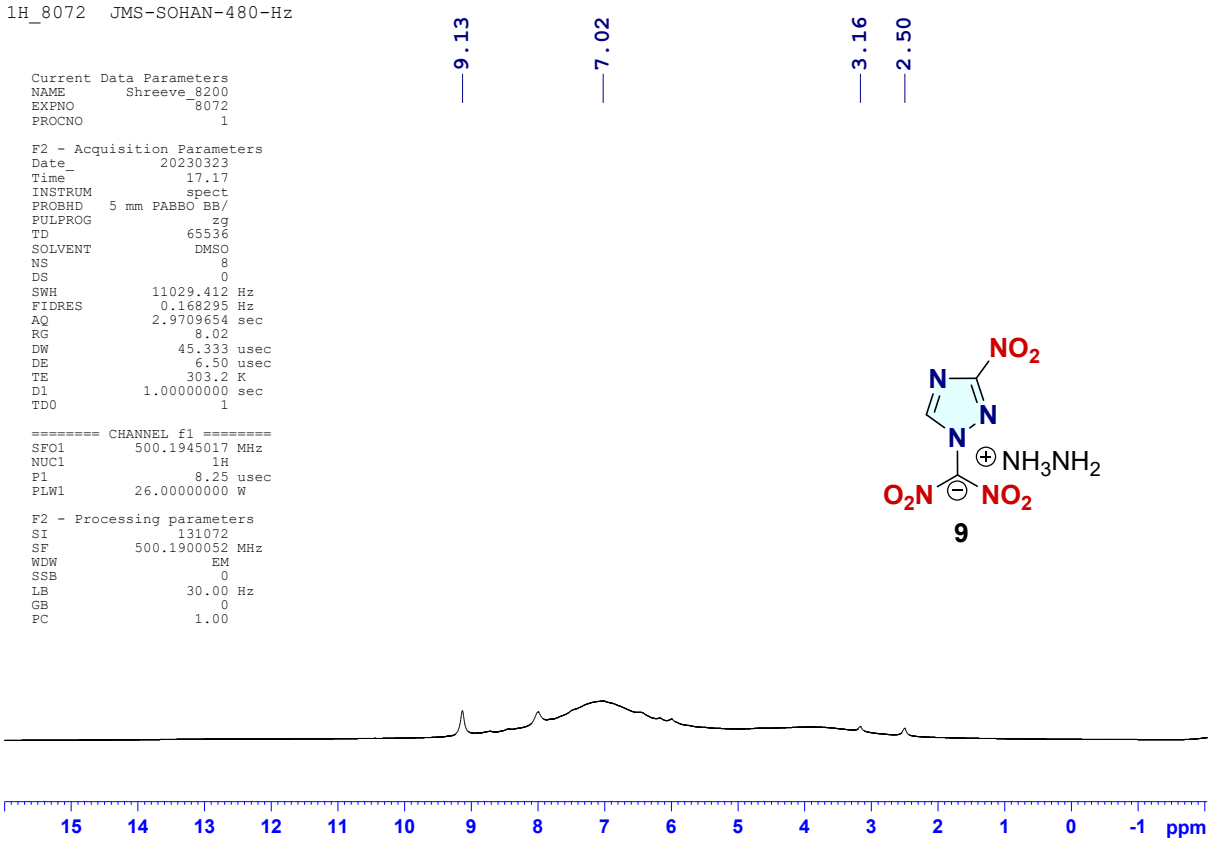



**Fig. S20**: $^{1}$H NMR Spectrum of Compound **9** (500.19 MHz).

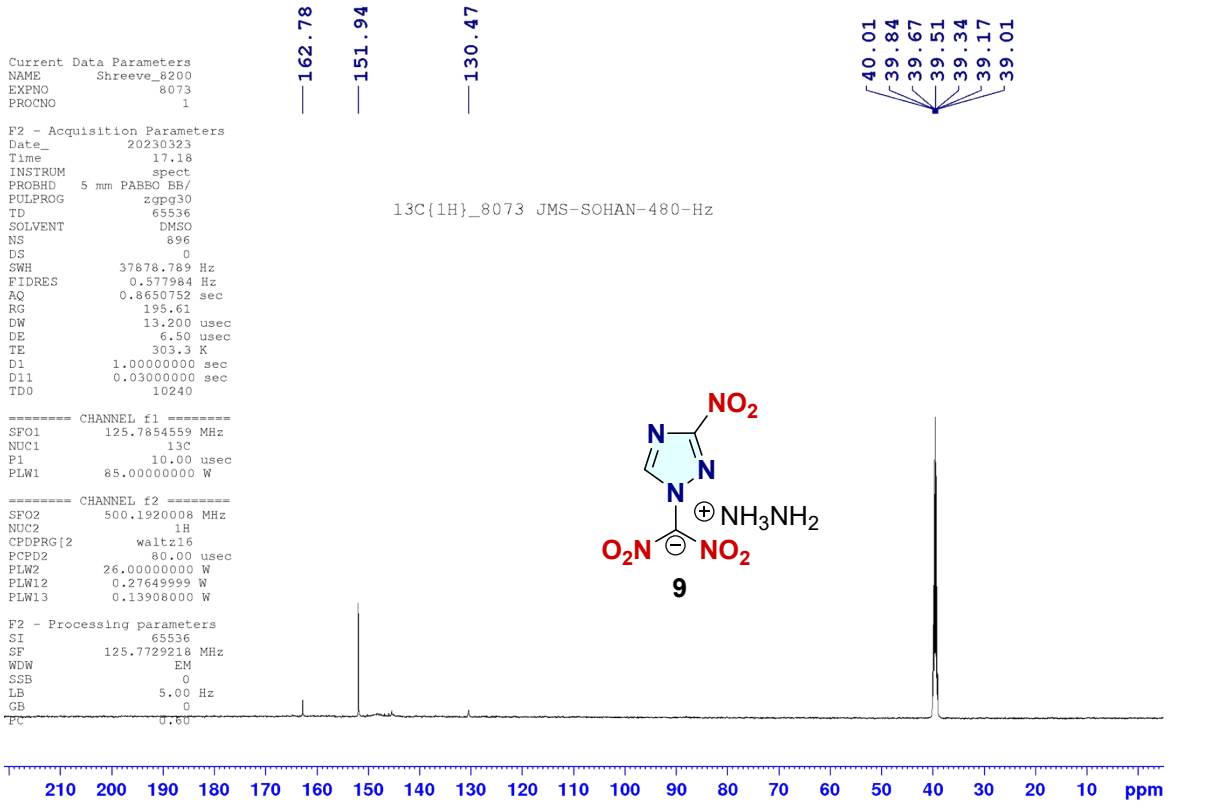



**Fig. S21**: $^{13}$C NMR Spectrum of Compound **9** (125.77 MHz).

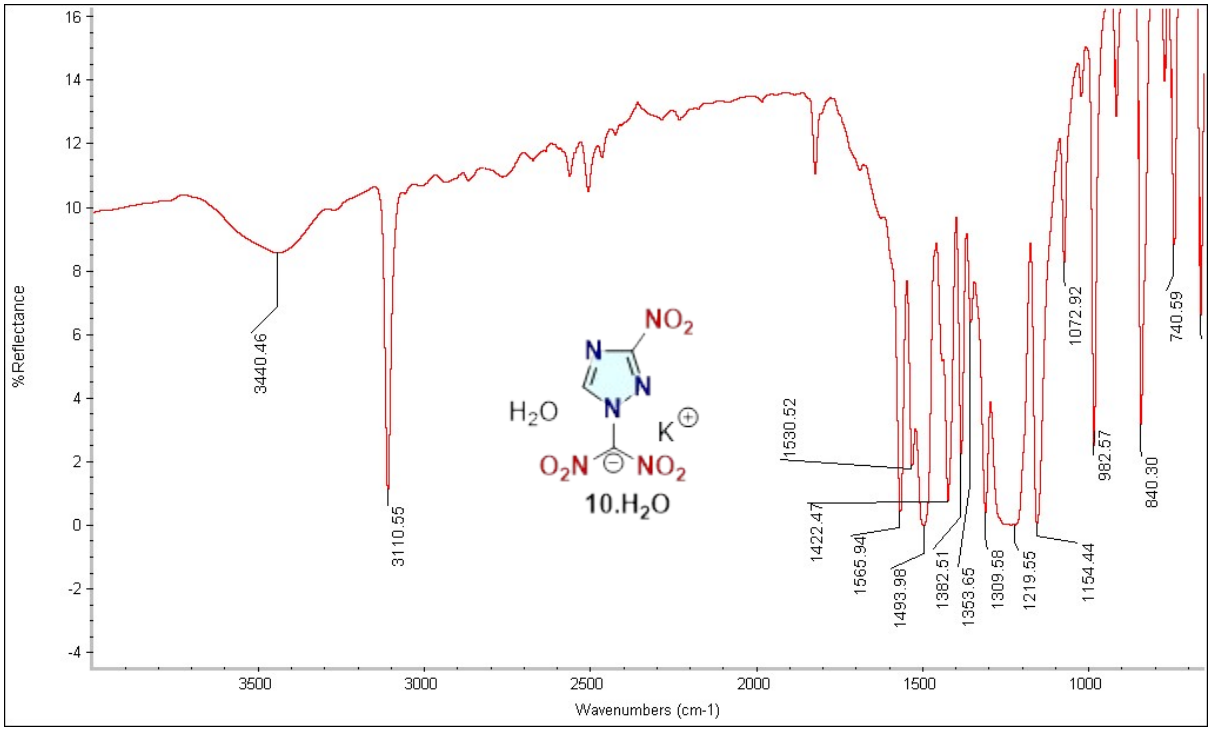



**Fig. S22:** FTIR-Spectrum of Compound **10.$H_2O$**.

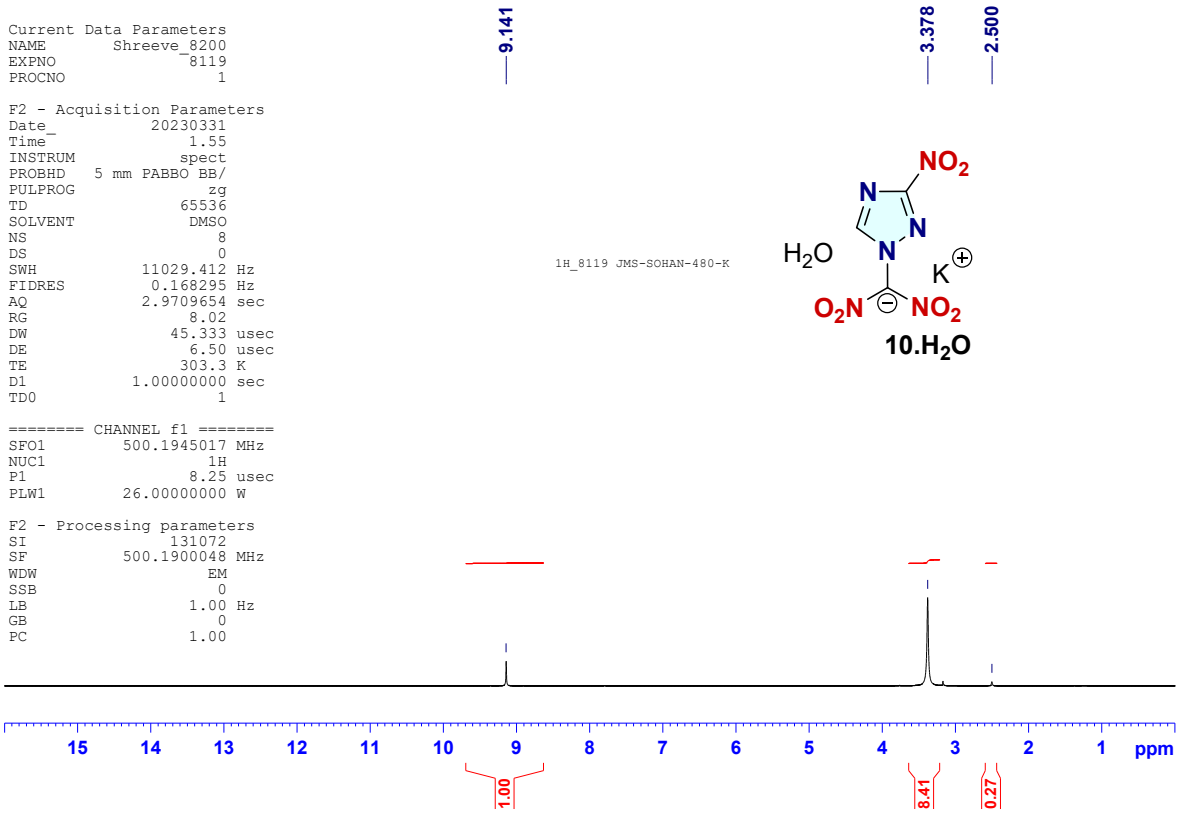



**Fig. S23**: $^1$H NMR Spectrum of Compound **10.$H_2O$** (500.19 MHz).

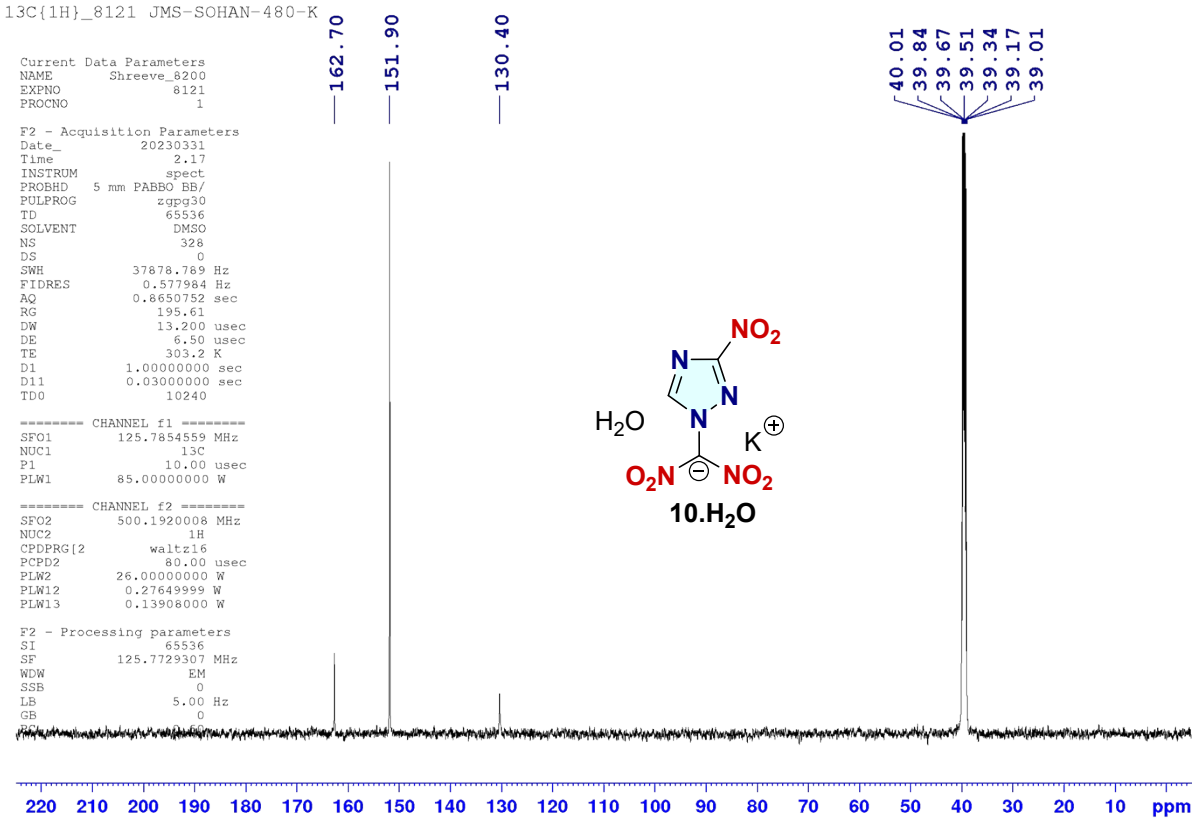



**Fig. S24**: $^{13}$C NMR Spectrum of Compound **10.H$_2$O** (125.77 MHz).

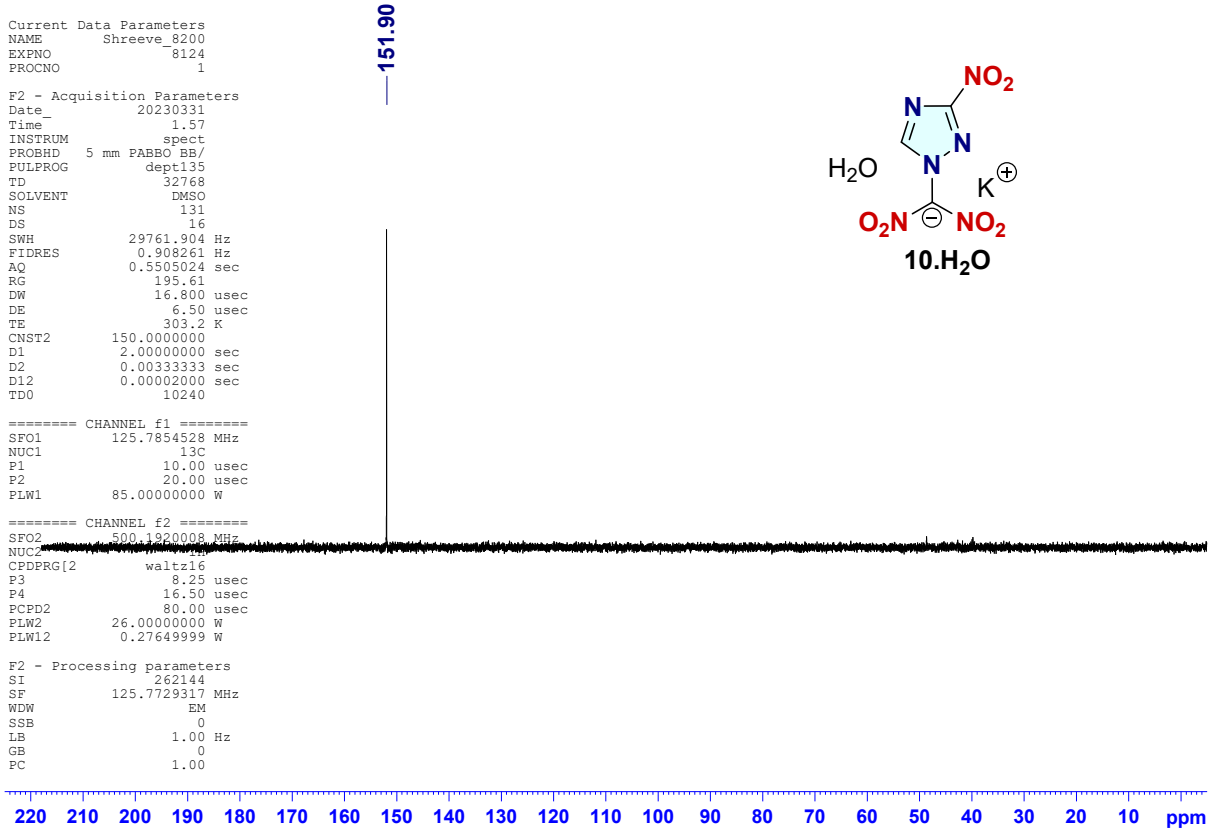



**Fig. S25**: $^{13}$C DEPT NMR Spectrum of Compound **10·H$_2$O** (125.77 MHz).

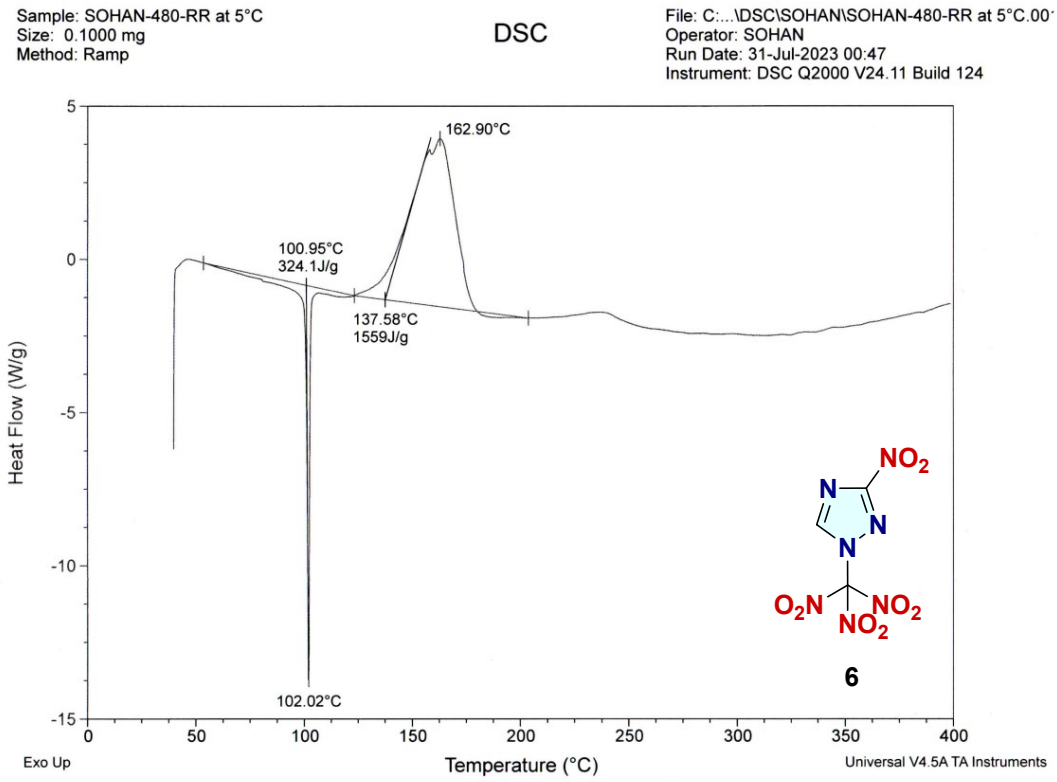



**Fig. S26:** DSC of compound **6** at 5 °C $min^{-1}$

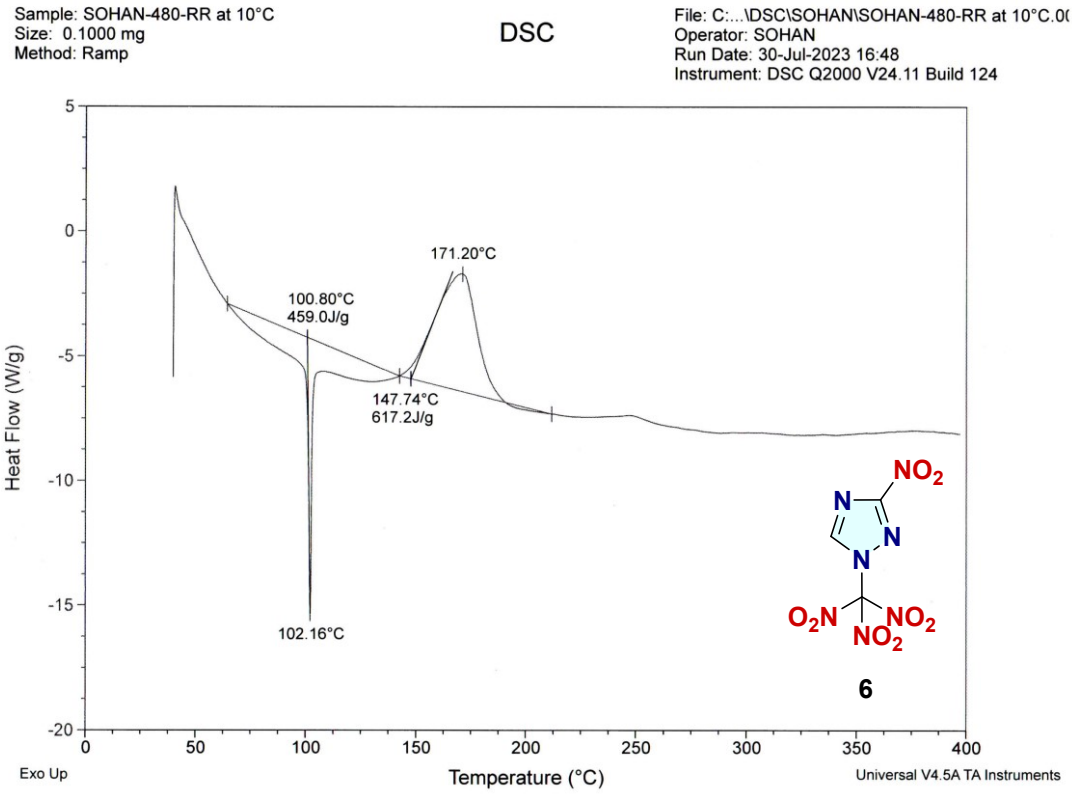



**Fig. S27:** DSC of compound **6** at 10 °C $min^{-1}$

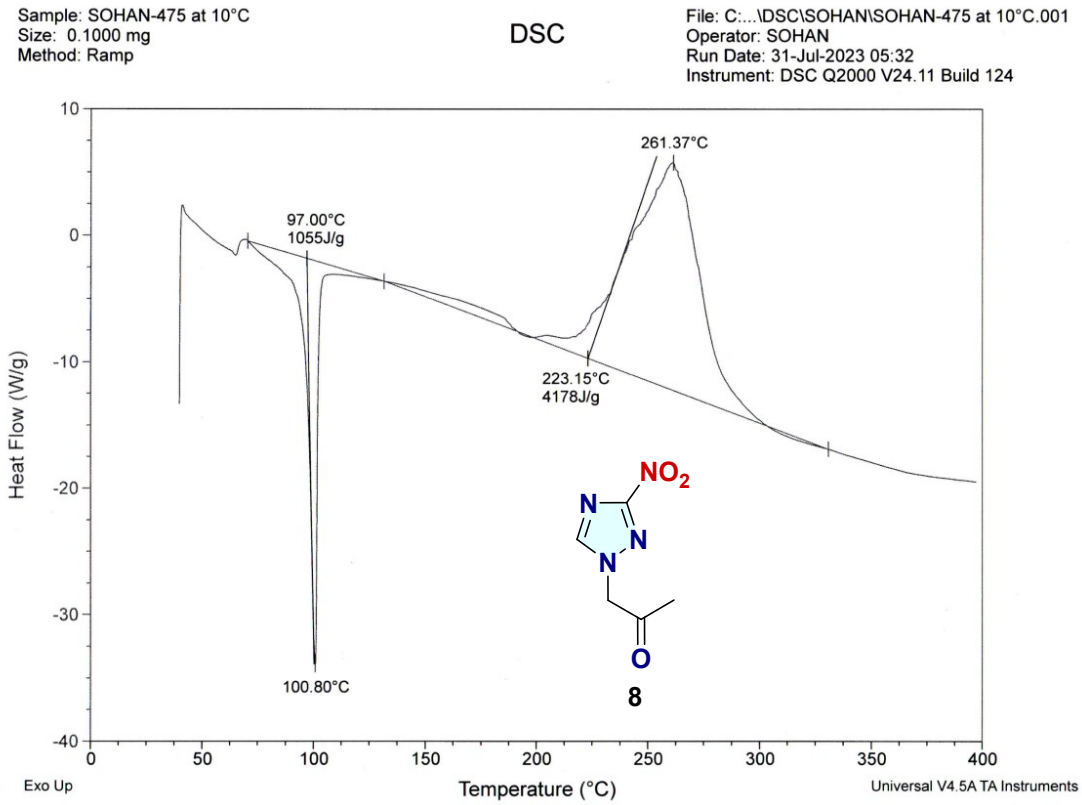



**Fig. S28:** DSC of compound **9** at 10 °C min$^{-1}$

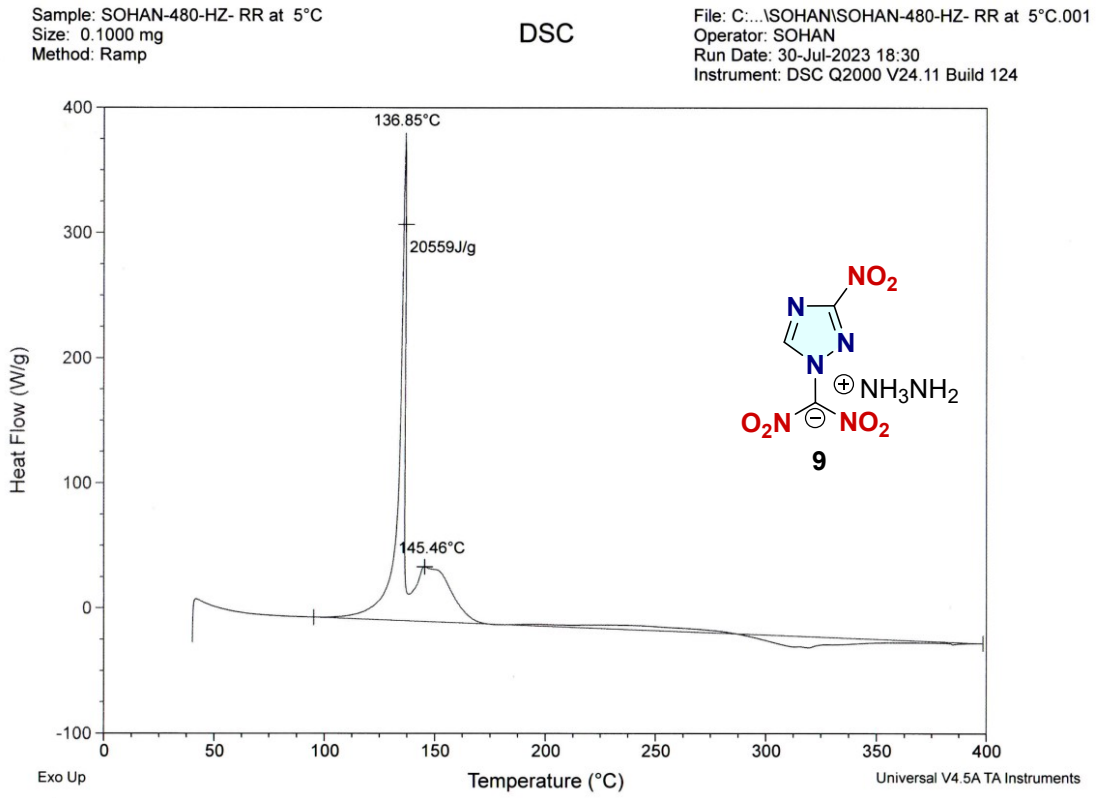



**Fig. S29:** DSC of compound **9** at 5 °C min$^{-1}$

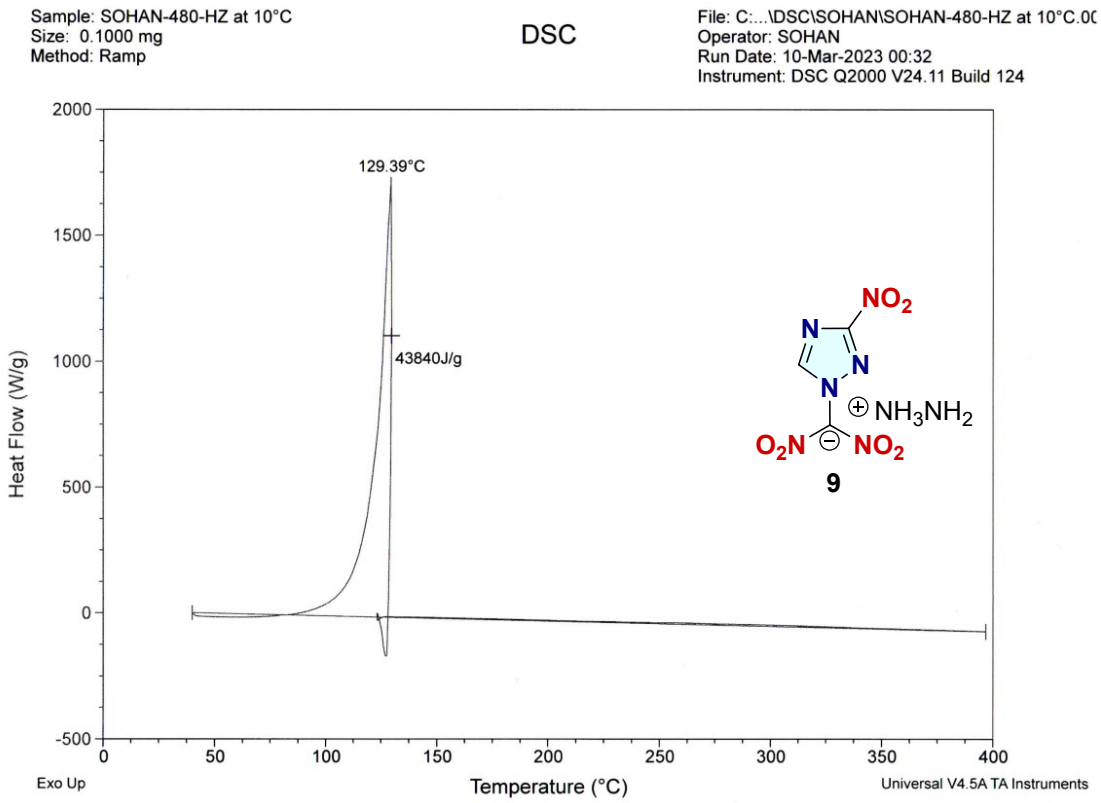



**Fig. S30:** DSC of compound **9** at 10 °C min$^{-1}$

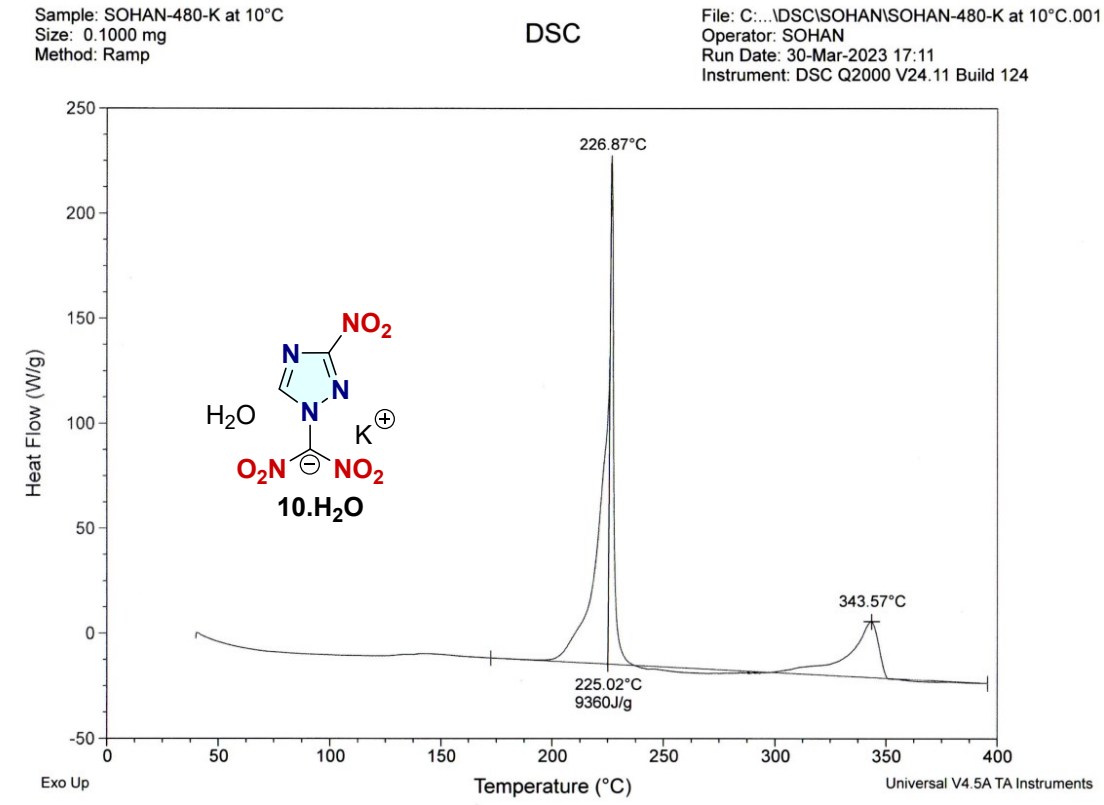



**Fig. S31:** DSC of compound **10** at 10 °C min$^{-1}$

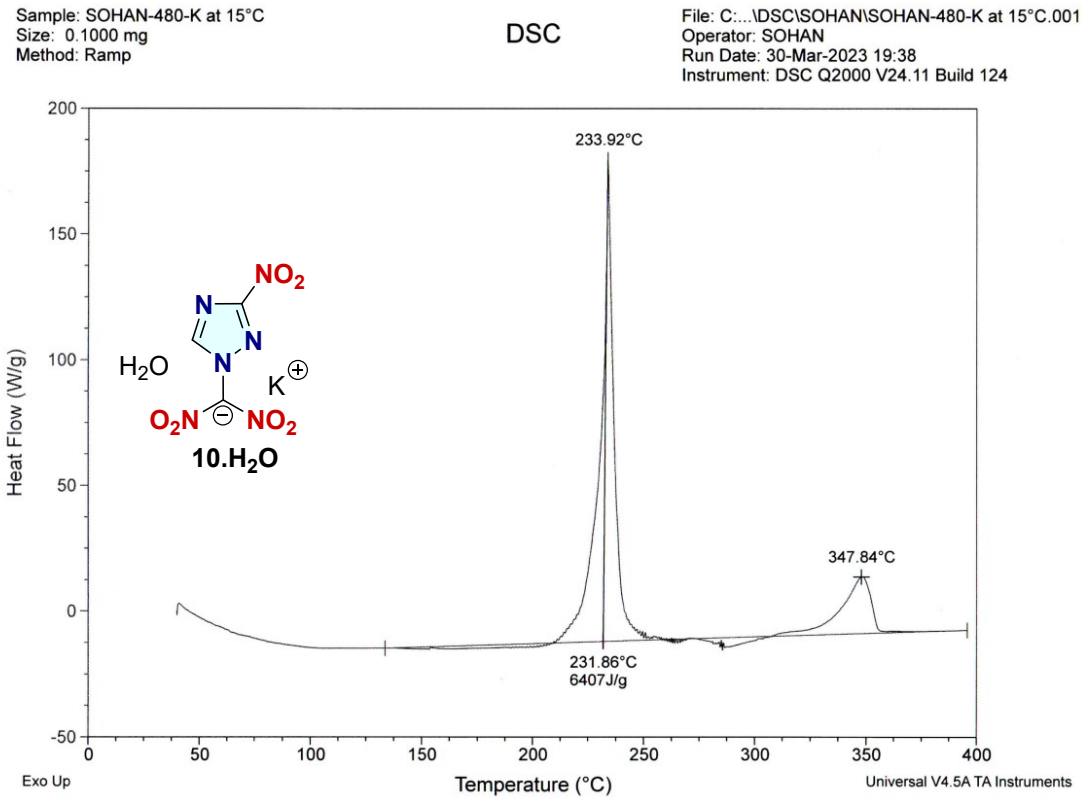



**Fig. S32:** DSC of compound **10** at 15 °C min$^{-1}$

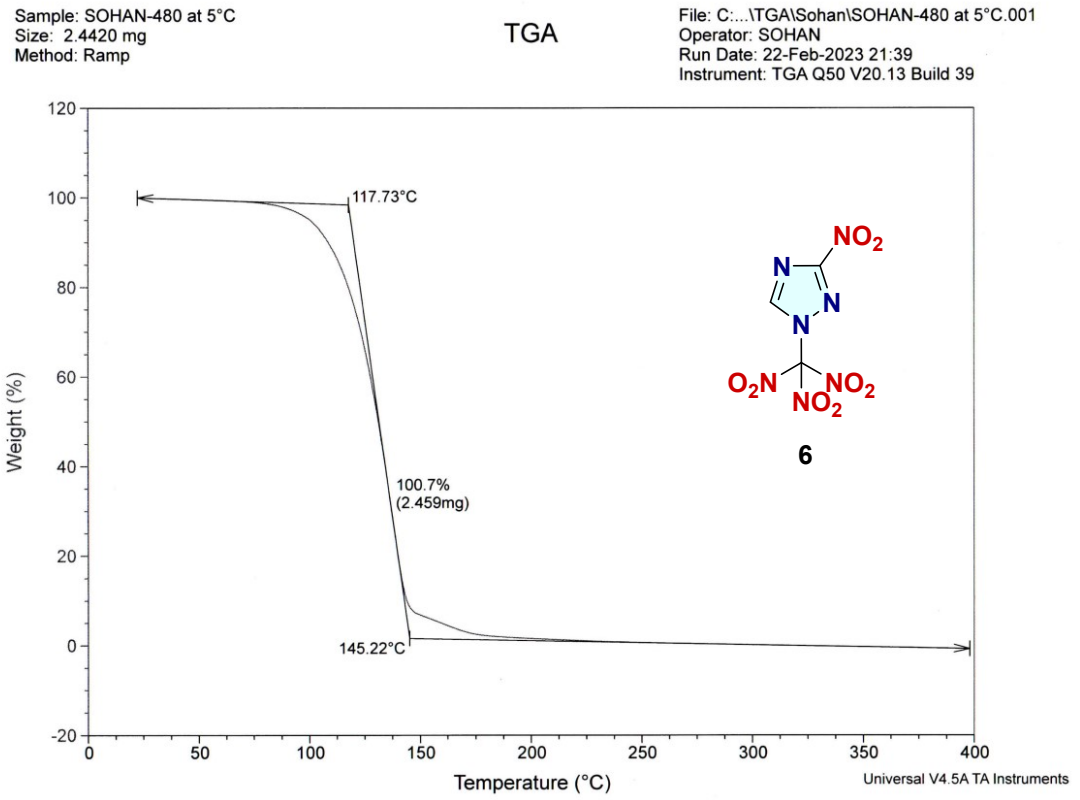



**Fig. S33:** TGA of compound **6** at 5 °C min$^{-1}$

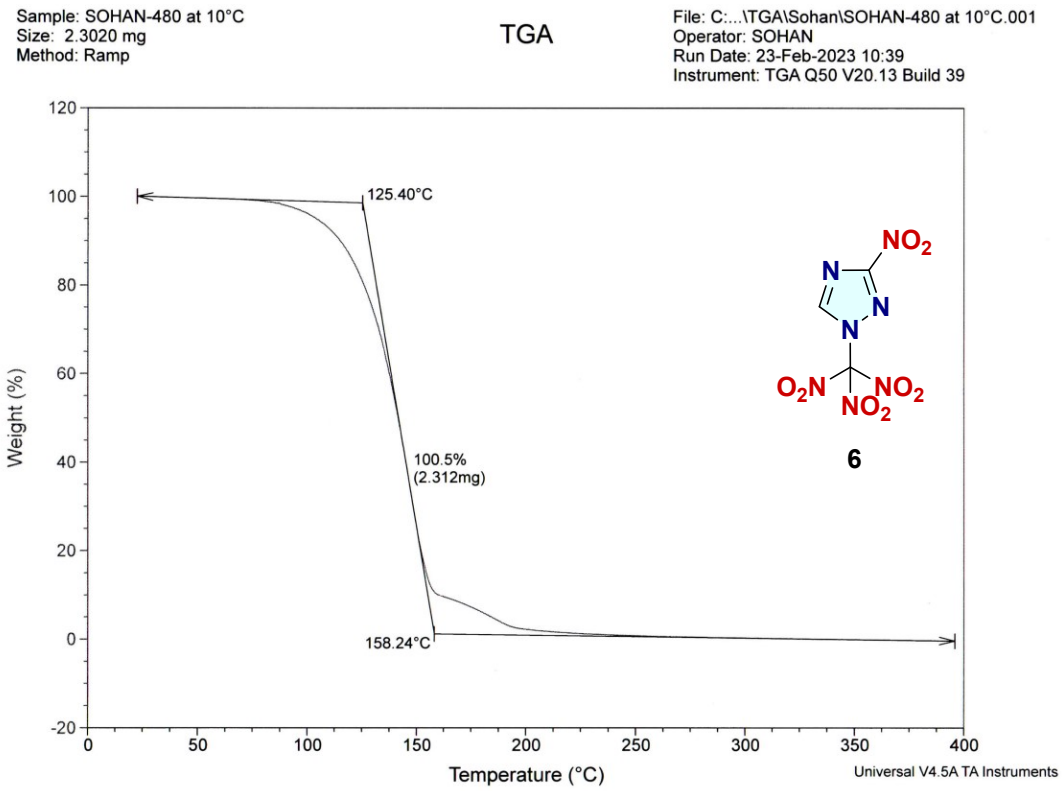



**Fig. S34:** TGA of compound **6** at 10 °C min$^{-1}$

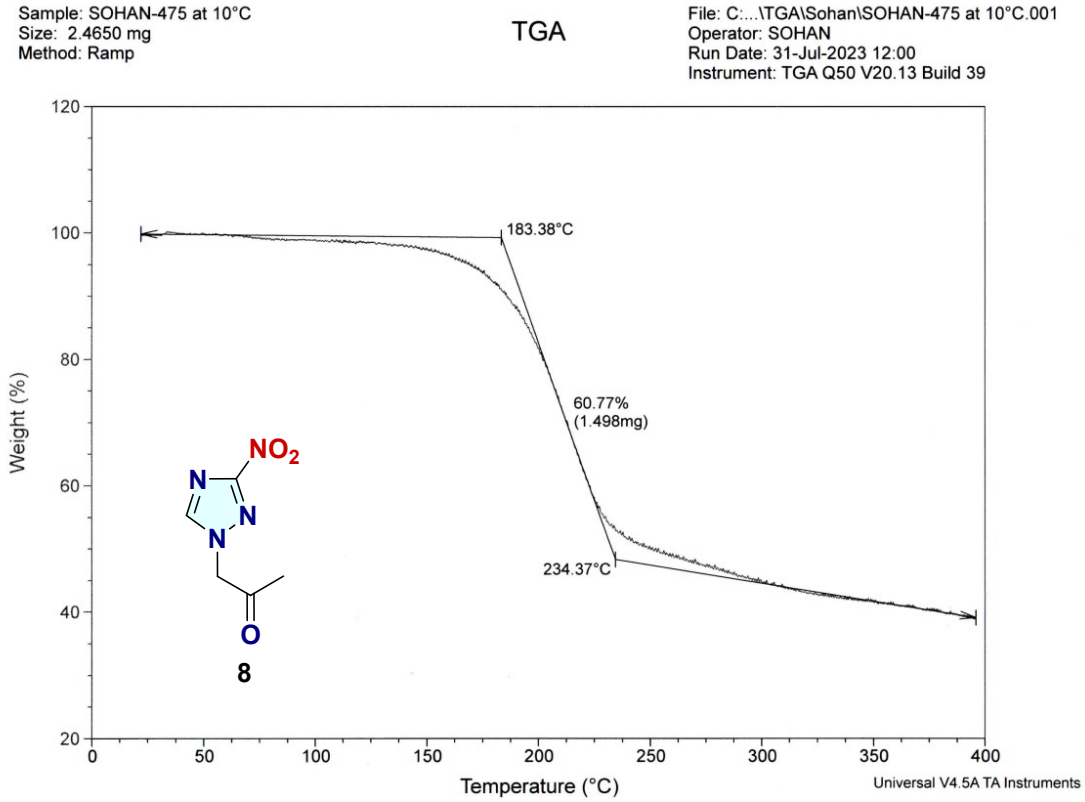



**Fig. S35:** TGA of compound **8** at 10 °C min$^{-1}$

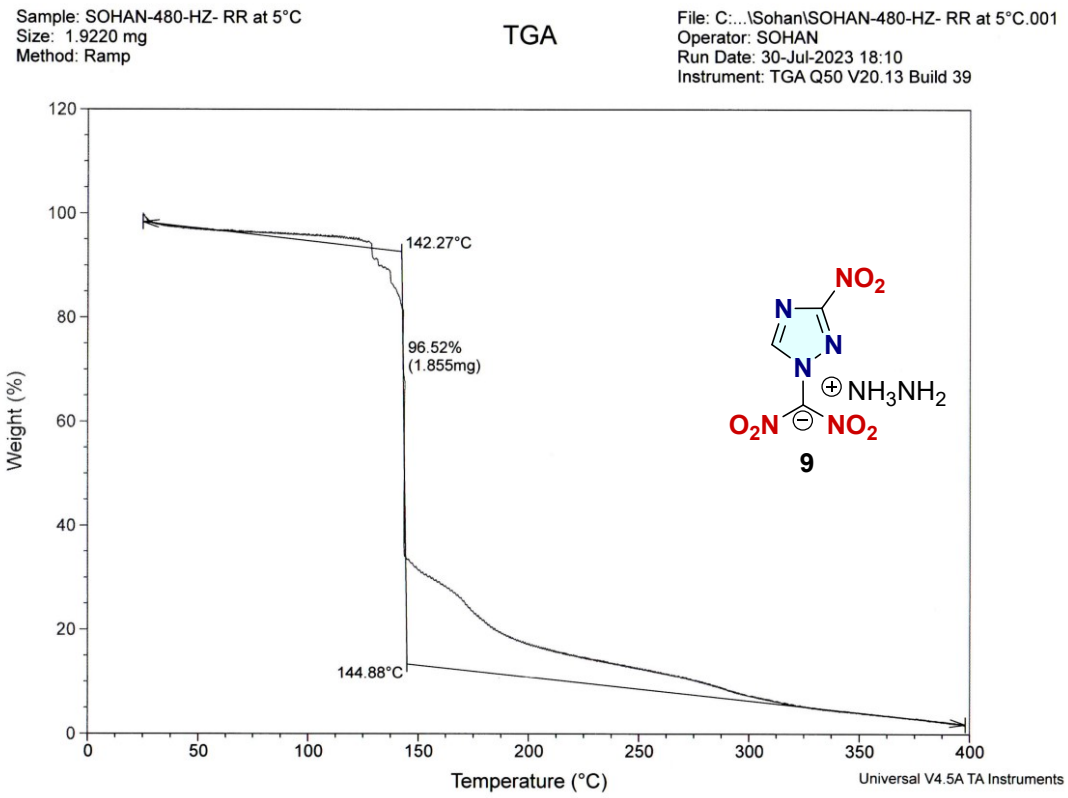



**Fig. S36:** TGA of compound **9** at 5 °C $min^{-1}$

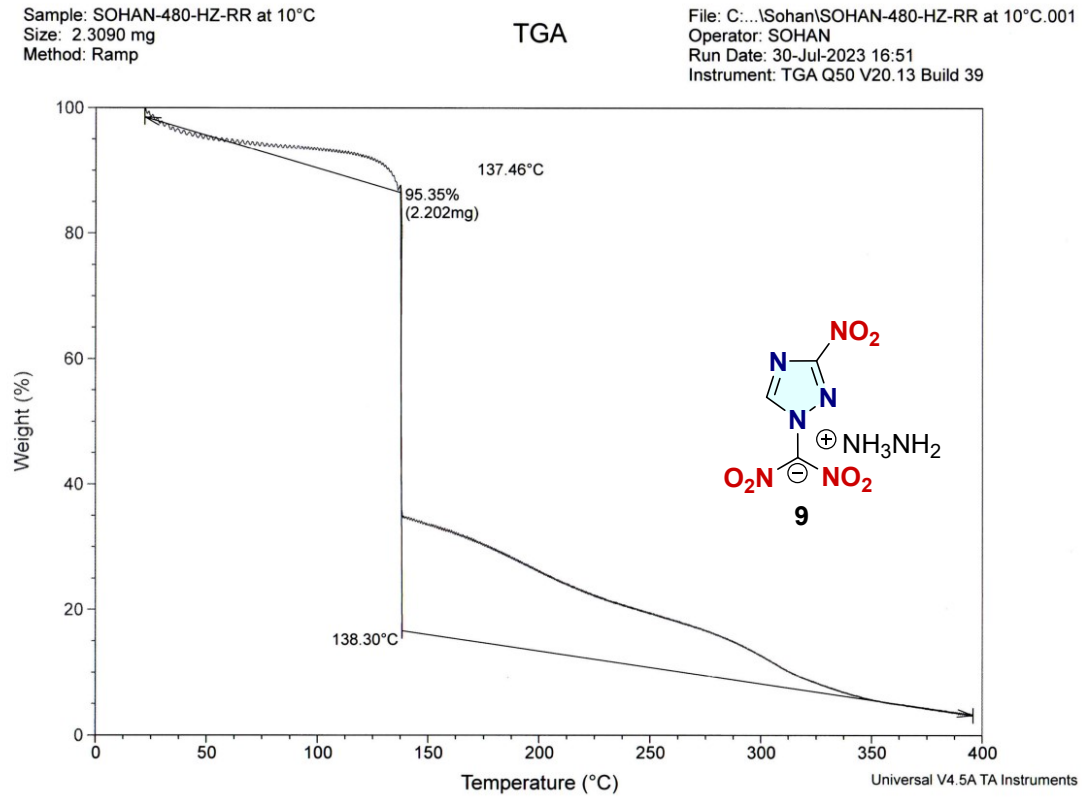



**Fig. S37:** TGA of compound **9** at 10 °C $min^{-1}$

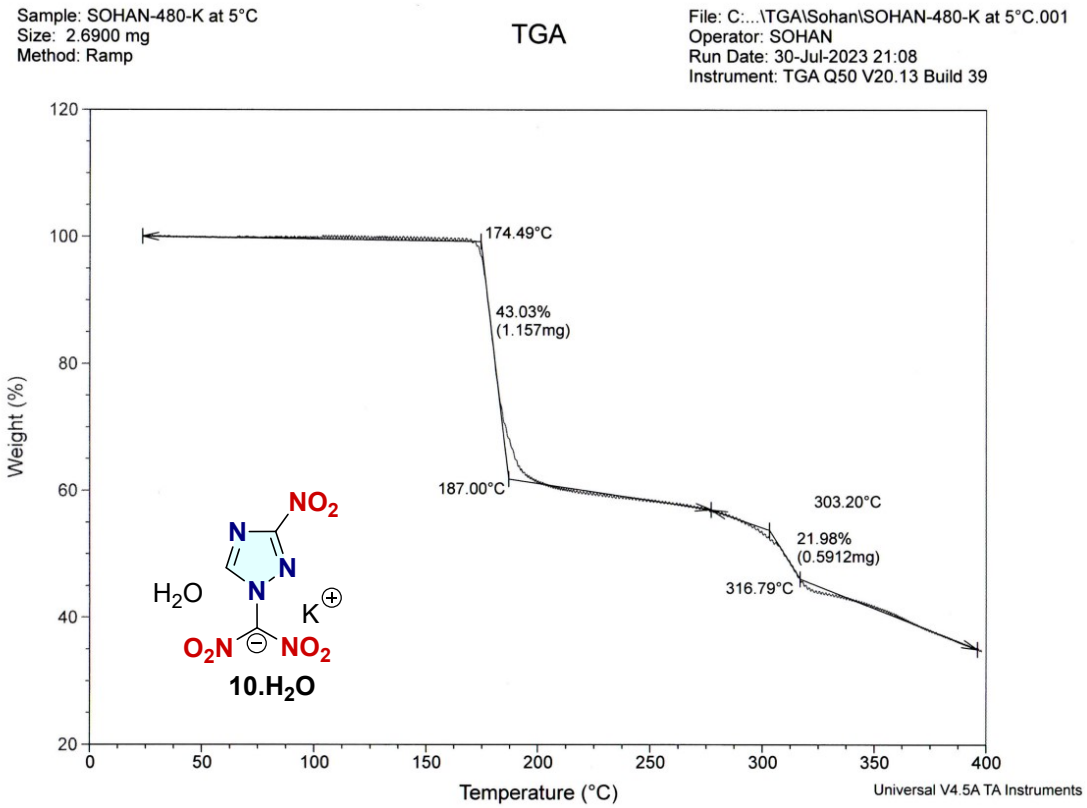



**Fig. S38:** TGA of compound **10.$H_2O$** at 5 °C $min^{-1}$

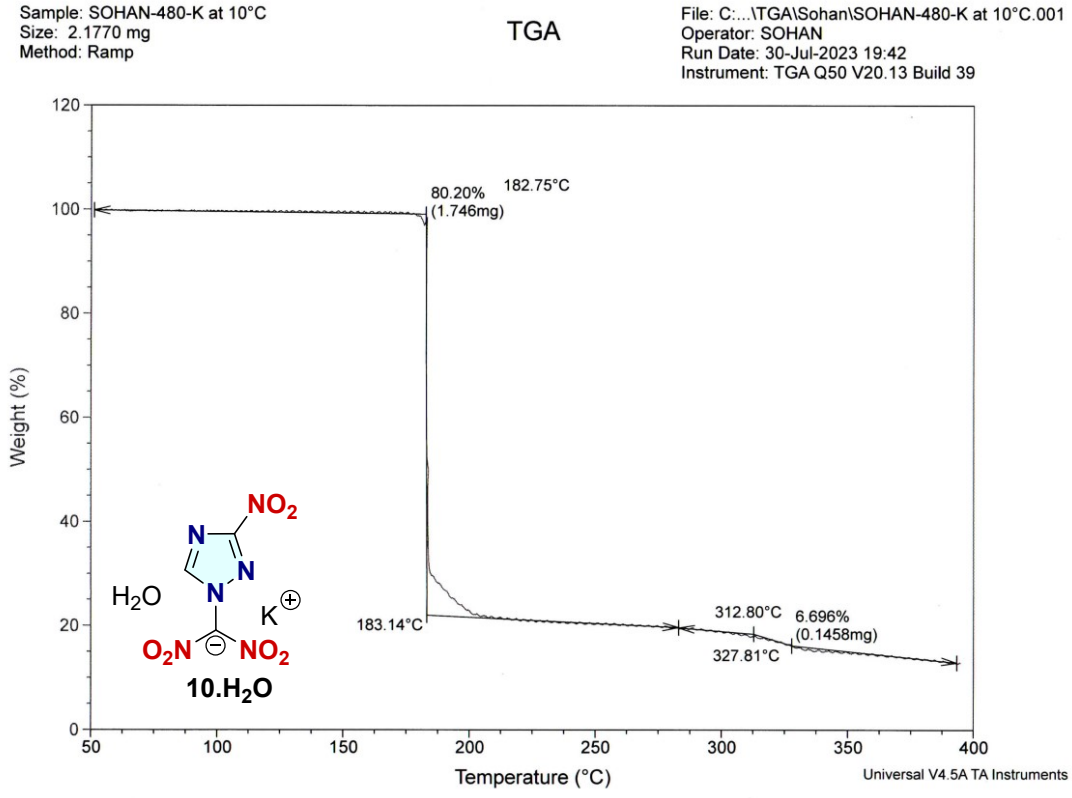



**Fig. S39:** TGA of compound **10.$H_2O$** at 10 °C $min^{-1}$

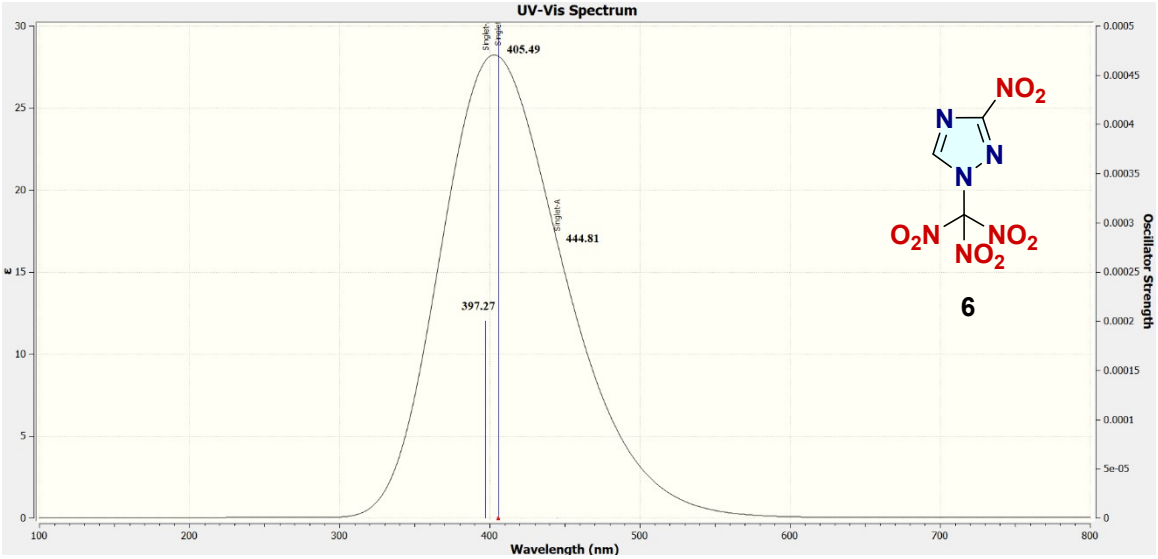
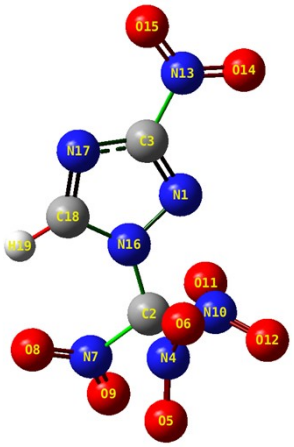



**Fig. S40**: Predicted UV-Visible spectrum of **6** at B3LYP/6-311++G(d,p) level.

**Table S14.** Cartesian coordinates (in Å) for optimized structure of compound **6** obtained using the B3LYP/6-311++G(d,p) level of theory

| | |
|---|---|
| Zero-point correction= | 0.094403 (Hartree/Particle) |
| Thermal correction to Energy= | 0.109684 |
| Thermal correction to Enthalpy= | 0.110628 |
| Thermal correction to Gibbs Free Energy= | 0.048625 |
| Sum of electronic and zero-point Energies= | -1099.701546 |
| Sum of electronic and thermal Energies= | -1099.686265 |
| Sum of electronic and thermal Enthalpies= | -1099.685321 |
| Sum of electronic and thermal Free Energies= | -1099.747324 |



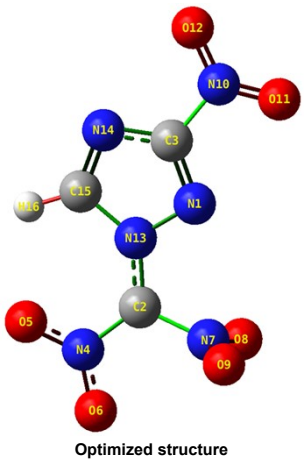
Optimized structure

| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | N | -2.189487 | 3.095441 | 0.599479 |
| 2 | C | -2.319869 | 0.835433 | -0.119287 |
| 3 | C | -1.405018 | 3.715717 | 1.439692 |
| 4 | N | -1.383990 | 0.631332 | -1.385548 |
| 5 | O | -1.537959 | -0.407870 | -1.980108 |
| 6 | O | -0.625956 | 1.540343 | -1.614973 |
| 7 | N | -2.472253 | -0.577199 | 0.504398 |
| 8 | O | -1.524571 | -0.936966 | 1.176068 |
| 9 | O | -3.468829 | -1.191052 | 0.229770 |
| 10 | N | -3.726162 | 1.301964 | -0.626890 |
| 11 | O | -4.546548 | 1.421726 | 0.247527 |
| 12 | O | -3.833753 | 1.479871 | -1.814106 |
| 13 | N | -1.489879 | 5.180319 | 1.609831 |
| 14 | O | -2.329035 | 5.757867 | 0.943002 |
| 15 | O | -0.710319 | 5.674347 | 2.402280 |
| 16 | N | -1.801367 | 1.797913 | 0.773622 |
| 17 | N | -0.526646 | 2.953483 | 2.135396 |
| 18 | C | -0.769690 | 1.750046 | 1.698713 |
| 19 | H | -0.280677 | 0.837441 | 1.991892 |

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

**Table S15.** Cartesian coordinates (in Å) for optimized structure of compound **6-D1** obtained using the B3LYP/6-311++G(d,p) level of theory

```
Zero-point correction=                           0.079828 (Hartree/Particle)
Thermal correction to Energy=                    0.092660
Thermal correction to Enthalpy=                  0.093604
Thermal correction to Gibbs Free Energy=         0.034006
Sum of electronic and zero-point Energies=          -894.530651
Sum of electronic and thermal Energies=             -894.517819
Sum of electronic and thermal Enthalpies=           -894.516875
Sum of electronic and thermal Free Energies=        -894.576473
```



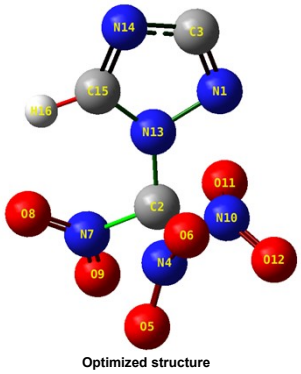
Optimized structure

| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | N | -2.204543 | 2.928810 | 0.546632 |
| 2 | C | -2.755684 | 0.667274 | 0.265800 |
| 3 | C | -1.276908 | 3.527315 | 1.247707 |
| 4 | N | -2.597797 | -0.725372 | 0.446627 |
| 5 | O | -1.661970 | -1.096796 | 1.161143 |
| 6 | O | -3.412156 | -1.444582 | -0.125935 |
| 7 | N | -3.868822 | 1.119666 | -0.590401 |
| 8 | O | -4.910405 | 1.355436 | -0.015091 |
| 9 | O | -3.623205 | 1.201659 | -1.774807 |
| 10 | N | -1.157007 | 4.998811 | 1.237504 |
| 11 | O | -1.982843 | 5.606112 | 0.580770 |
| 12 | O | -0.240921 | 5.466267 | 1.887590 |
| 13 | N | -1.957349 | 1.614726 | 0.835206 |
| 14 | N | -0.441909 | 2.736995 | 1.971018 |
| 15 | C | -0.867093 | 1.535269 | 1.714126 |
| 16 | H | -0.488905 | 0.597437 | 2.080752 |

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

**Table S16.** Cartesian coordinates (in Å) for optimized structure of compound **6-D2** obtained using the B3LYP/6-311++G(d,p) level of theory

```
Zero-point correction=                           0.079459 (Hartree/Particle)
Thermal correction to Energy=                    0.092022
Thermal correction to Enthalpy=                  0.092966
Thermal correction to Gibbs Free Energy=         0.038198
Sum of electronic and zero-point Energies=          -894.474789
Sum of electronic and thermal Energies=             -894.462226
Sum of electronic and thermal Enthalpies=           -894.461282
Sum of electronic and thermal Free Energies=        -894.516051
```



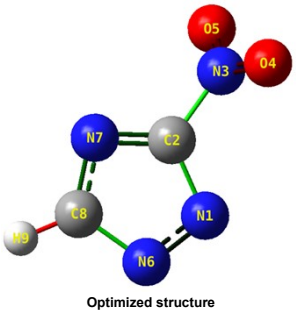
Optimized structure

| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | N | -2.699458 | 2.998231 | 1.083668 |
| 2 | C | -2.351270 | 0.898184 | -0.038995 |
| 3 | C | -2.042693 | 3.554634 | 2.044895 |
| 4 | N | -1.327206 | 1.070877 | -1.245153 |
| 5 | O | -1.273005 | 0.145162 | -2.019512 |
| 6 | O | -0.715745 | 2.110022 | -1.254823 |
| 7 | N | -2.291289 | -0.615797 | 0.316414 |
| 8 | O | -1.344899 | -0.933820 | 1.010666 |
| 9 | O | -3.139789 | -1.325336 | -0.155915 |
| 10 | N | -3.783386 | 1.215480 | -0.583588 |
| 11 | O | -4.668609 | 1.011495 | 0.208126 |
| 12 | O | -3.847177 | 1.621278 | -1.718096 |
| 13 | N | -2.065854 | 1.747687 | 1.037354 |
| 14 | N | -1.050287 | 2.869688 | 2.635802 |
| 15 | C | -1.054103 | 1.735512 | 1.980288 |
| 16 | H | -0.401020 | 0.893386 | 2.131947 |

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

**Table S17.** Cartesian coordinates (in Å) for optimized structure of compound **6-D3** obtained using the B3LYP/6-311++G(d,p) level of theory

```
Zero-point correction=                           0.046512 (Hartree/Particle)
Thermal correction to Energy=                    0.052727
Thermal correction to Enthalpy=                  0.053671
Thermal correction to Gibbs Free Energy=         0.014508
Sum of electronic and zero-point Energies=            -446.130405
Sum of electronic and thermal Energies=               -446.124190
Sum of electronic and thermal Enthalpies=             -446.123246
Sum of electronic and thermal Free Energies=          -446.162409
```



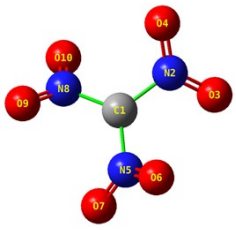
Optimized structure

| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | N | -2.628669 | 3.043529 | 1.583488 |
| 2 | C | -1.301230 | 3.470423 | 1.367245 |
| 3 | N | -1.018970 | 4.846438 | 0.997260 |
| 4 | O | -1.518251 | 5.214377 | -0.052584 |
| 5 | O | -0.332367 | 5.499355 | 1.759576 |
| 6 | N | -2.521423 | 1.798775 | 1.866291 |
| 7 | N | -0.376274 | 2.536527 | 1.498039 |
| 8 | C | -1.136862 | 1.488433 | 1.811194 |
| 9 | H | -0.765378 | 0.492179 | 2.004236 |

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

**Table S18.** Cartesian coordinates (in Å) for optimized structure of compound **6-D4** obtained using the B3LYP/6-311++G(d,p) level of theory

```
Zero-point correction=                           0.040184 (Hartree/Particle)
Thermal correction to Energy=                    0.049347
Thermal correction to Enthalpy=                  0.050291
Thermal correction to Gibbs Free Energy=         0.003113
Sum of electronic and zero-point Energies=            -653.449476
Sum of electronic and thermal Energies=               -653.440313
Sum of electronic and thermal Enthalpies=             -653.439369
Sum of electronic and thermal Free Energies=          -653.486548
```



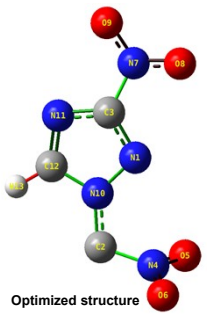
Optimized structure

| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.534445 | 0.647264 | -0.462957 |
| 2 | N | -1.391242 | 1.432758 | -0.885875 |
| 3 | O | -0.430582 | 0.801808 | -1.287549 |
| 4 | O | -1.511242 | 2.640799 | -0.795107 |
| 5 | N | -2.334958 | -0.567435 | 0.303824 |
| 6 | O | -1.486256 | -0.514249 | 1.174986 |
| 7 | O | -3.036816 | -1.513354 | -0.003794 |
| 8 | N | -3.876678 | 1.075894 | -0.805357 |
| 9 | O | -4.714225 | 0.954557 | 0.069923 |
| 10 | O | -4.026139 | 1.512077 | -1.932079 |

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

**Table S19.** Cartesian coordinates (in Å) for optimized structure of compound **6-D5** obtained using the B3LYP/6-311++G(d,p) level of theory

```
Zero-point correction=                           0.065132 (Hartree/Particle)
Thermal correction to Energy=                    0.074744
Thermal correction to Enthalpy=                  0.075688
Thermal correction to Gibbs Free Energy=         0.027120
Sum of electronic and zero-point Energies=            -689.483828
Sum of electronic and thermal Energies=               -689.474215
Sum of electronic and thermal Enthalpies=             -689.473271
Sum of electronic and thermal Free Energies=          -689.521839
```



Optimized structure

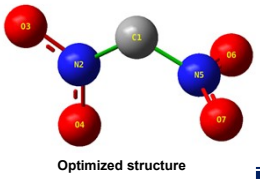
| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | N | -2.260558 | 3.010776 | 0.534681 |
| 2 | C | -2.834791 | 0.613567 | 0.332950 |
| 3 | C | -1.274809 | 3.545249 | 1.248653 |
| 4 | N | -3.993855 | 1.026510 | -0.397262 |
| 5 | O | -4.921369 | 1.582606 | 0.206686 |
| 6 | O | -4.069620 | 0.670551 | -1.581790 |

| | | | | |
|---|---|---|---|---|
| 7 | N | -1.019555 | 4.959847 | 1.241857 |
| 8 | O | -1.746647 | 5.672618 | 0.544659 |
| 9 | O | -0.085306 | 5.381512 | 1.933752 |
| 10 | N | -2.133001 | 1.679357 | 0.830334 |
| 11 | N | -0.517357 | 2.686637 | 1.979368 |
| 12 | C | -1.065806 | 1.531153 | 1.703345 |
| 13 | H | -0.774041 | 0.560497 | 2.069406 |

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

**Table S20.** Cartesian coordinates (in Å) for optimized structure of compound **6-D6** obtained using the B3LYP/6-311++G(d,p) level of theory

```
Zero-point correction=                           0.025956 (Hartree/Particle)
Thermal correction to Energy=                    0.032112
Thermal correction to Enthalpy=                  0.033057
Thermal correction to Gibbs Free Energy=        -0.006115
Sum of electronic and zero-point Energies=           -448.407158
Sum of electronic and thermal Energies=              -448.401002
Sum of electronic and thermal Enthalpies=            -448.400057
Sum of electronic and thermal Free Energies=         -448.439229
```



Optimized structure

| Center Number | Atomic Symbol | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|
| 1 | C | -2.553789 | 0.850542 | 0.051801 |
| 2 | N | -2.357987 | -0.526573 | 0.233456 |
| 3 | O | -1.480846 | -0.853775 | 1.070814 |
| 4 | O | -2.987399 | -1.385476 | -0.435803 |
| 5 | N | -3.822511 | 1.089488 | -0.597723 |
| 6 | O | -4.828152 | 1.182086 | 0.115771 |
| 7 | O | -3.817408 | 1.342699 | -1.804418 |

Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

**Table S21**. Comparison of the enthalpy of sublimation (kJ/mol) of compound 6.

| Compound | Method A | Method B | Method C |
|---|---|---|---|
| **6** | 70.31 | 122.87 | 114.17 |

[a] Method A: Trouton's rule, Refs. 3-4; Method B: Ref. 10; Method C: Ref. 11.

**Method A:** $\Delta H_{sub} = 0.188 \times T/kJmol^{-1}K^{-1}$

where, *T*, is either the melting point (mp) or the decomposition temperature ($T_d$), when melting does not occur before decomposition.

**Method B**: $\Delta H_{sub}$ (kJ $mol^{-1}$) = $0.15 \times T_m(K) + 3.27 \times [H] + 5.30 \times [N] + 3.30 \times [O]$.

Where, $T_m$ is he melting temperature, and [H], [N] and [O] are the number of hydrogen, nitrogen and oxygen atoms present in the molecule, respectively.

**Method C:** $\Delta H_{sub} = a(SA)^2 + b\sqrt{(\sigma^2_{tot}\upsilon)} + c$

Where, *a*, *b* and *c* are fitting parameters, SA is the surface area of the 0.001 electron $bohr^{-3}$ isosurface of the electrostatic potential of the molecules, $\sigma^2_{tot}$ is the measure of

variability of electronic potential on the surface, and υ is the degree of balance between the positive and negative charges on the isosurface. For compound 6: SA = 223.12533 $Å^2$; $\sigma^2_{tot}$ = 255.31032 $(kcal/mol)^2$; υ = 0.17475149.

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