# Harnessing Triazole-Oxadiazole-Trinitromethyl Moieties in the Synthesis of Insensitive Energetic Material with Enhanced Detonation Performance

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## SUPPORTING INFORMATION

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## Experimental

### General Experimental

All the reactions were performed in an oven-dried round bottomed flask. Commercial grade solvents were distilled prior to use. Column chromatography was performed using silica gel (100-200 Mesh) with hexanes and ethyl acetate mixture. Thin layer chromatography (TLC) was performed on silica gel GF254 plates. Visualization of spots on TLC plate was accomplished with UV light (254 nm) and staining over $I_2$ chamber.

Proton and carbon nuclear magnetic resonance spectra ($^1$H NMR, $^{13}$C NMR) were recorded on 600 MHz ($^1$H NMR, 600 MHz; $^{13}$C NMR, 151 MHz; $^{15}$N NMR, 61 MHz; spectra were recorded with a JEOL JNM-ECZ-600R/M1) spectrometer, respectively. The chemical shift values (ppm) are expressed relative to the chemical shift of deuterated-solvent or to the external standard Liq.$NH_3$ without correction ($^{15}$N NMR). Data for $^1$H NMR are reported as follows: chemical shift (ppm), multiplicity (s = singlet; bs = broad singlet; d = doublet; bd = broad doublet; dd = doublet of doublet; dt = doublet of triplet; tt = triplet of triplet; t = triplet; bt= broad triplet; q = quartet; pent = pentet, m = multiplet), coupling constants *J* in (Hz), and integration. $^{13}$C NMR was reported in terms of chemical shift (ppm). Melting points and decomposition temperatures (DTA) were determined by DSC-TGA measurements. IR spectra were recorded on FT/IR spectrometer and are reported in $cm^{-1}$. High resolution mass spectra (HRMS) were obtained in ESI mode. X-ray data was collected at 295 K on a 'Bruker D8 VENTURE Photon III detector' diffractometer using Mo-Kα radiation (0.71073Å).

**Caution!** The trinitro-functionalized triazole-bis-1,2,4-oxadiazole compound is an energetic material and it tends to exploded or detonated under certain conditions such as impact, friction in the course of the research. Safety precautions including gloves, safety goggles, and face shields should be used all the time.

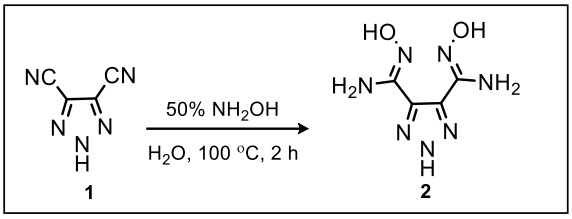
**Materials:** Unless otherwise noted, all the reagents were obtained commercially and used without purification. 4,5-Dicyano-2*H*-1,2,3-triazole, $Sc(OTf)_3$, trimethylorthoformate, 50% hydroxylamine, methyl vinyl ketone, acetonitrile ($CH_3CN$) were commercially available and used as received. Concentrated $H_2SO_4$ and fuming $HNO_3$ were commercially available and used for nitration.

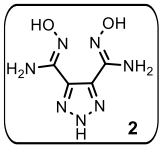
**Experimental Procedures:**

**Preparation of (4Z, 5Z)-*N'*4,*N'*5-dihydroxy-2*H*-1,2,3-triazole-4,5-bis(carboximidamide) (2):**[1]

2*H*-1,2,3-Triazole-4,5-dicarbonitrile (**1**, 6.0 g, 50.42 mmol) was dissolved in water (150 mL), and a hydroxylamine solution (50 wt% in $H_2O$, 6.9 mL, 226.9 mmol) was added dropwise at 0 °C. The reaction mixture was then refluxed at 100 °C for 2 h. The resulting solid was filtered and air-dried, yielding compound **2** (8.58 g) in 92% yield as colorless solid.

**Physical characterization data is exactly matching with the reported values for the respective compound 2.**

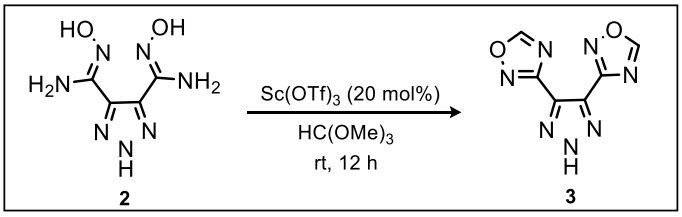


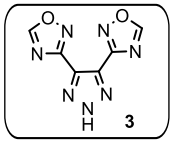




$^1$H NMR (600 MHz, DMSO–$d_6$): $\delta$ = 15.30 (bs), 9.94 (bs, 2H), 6.74 (bs, 4H). HRMS (ESI) for $C_4H_8N_7O_2^+$ $(M+H)^+$: calcd 186.0739, found 186.0745.

**Preparation of 4,5-di(1,2,4-oxadiazol-3-yl)-2*H*-1,2,3-triazole (3):**[2]

Bis-amidoxime **2** (200 mg, 1.08 mmol) was suspended in trimethyl orthoformate (0.8 mL), and $Sc(OTf)_3$ (200 mg, 0.22 mmol) was added at room temperature under an inert atmosphere. The resulting mixture was stirred for 12 h. After adding water, the resulting solid was filtered, washed with water, and air-dried to yield desired product **3** (188 mg) in 85% yield as colorless solid.

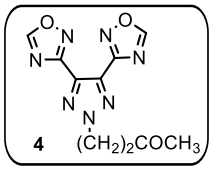



DSC–TGA (10 °C $min^{-1}$, °C): 183 °C ($T_d$-onset). $^1$H NMR (600 MHz, DMSO–$d_6$): $\delta$ = 16.58 (bs, 1H), 9.83 (s, 2H); $^{13}$C NMR (151 MHz, DMSO–$d_6$): $\delta$ = 167.8, 160.2, 133.3 ppm. IR(Neat) $\upsilon_{max}$ 3188, 3108, 2163, 2030, 1577, 1461, 1340, 1222, 1111, 922, 819, 746 $cm^{-1}$. HRMS (ESI) for $C_6H_4N_7O_2^+$ $(M+H)^+$: calcd 206.0426, found 206.0422.

**Preparation of 4-(4,5-di(1,2,4-oxadiazol-3-yl)-2*H*-1,2,3-triazol-2-yl)butan-2-one (4):**[4]

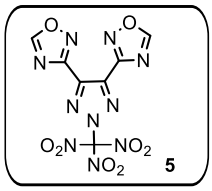
Compound **3** (150 mg, 0.73 mmol) was dissolved in $CH_3CN$ (4.0 mL), followed by the addition of triethylamine (220 mg, 2.19 mmol). Methyl vinyl ketone (102 mg, 1.46 mmol) was then added to the solution, and the mixture was stirred for 5 h at room temperature in the absence of light. The resulting precipitate was filtered, washed with $CH_3CN$, and air-dried to obtain compound **4** (196 mg) in 98% yield as colorless solid.




DSC–TGA (10 °C $min^{-1}$, °C): 167 °C ($T_d$); $^1$H NMR (600 MHz, $CD_3CN$): $\delta$ = 9.12 (s, 2H), 4.81 (t, $J$ = 6.6 Hz, 2H), 3.27 (t, $J$ = 6.6 Hz, 2H), 2.16 (s, 3H); $^{13}$C NMR (151 MHz, $CD_3CN$): $\delta$ = 206.2, 167.6, 161.5, 135.7, 51.7, 42.1, 30.1 ppm. IR(Neat) $\upsilon_{max}$ 3099, 3015, 2025, 1867, 1718, 1598, 1410, 1328, 1185, 1018, 903, 890, 774 $cm^{-1}$. HRMS (ESI) for $C_{10}H_{10}N_7O_3^+$ $(M+H)^+$: calcd 276.0845, found 276.0841.

**Preparation of 3,3′-(2-(trinitromethyl)-2*H*-1,2,3-triazole-4,5-diyl)bis(1,2,4-oxadiazole) (5):**[4, 5]

Compound **4** (840 mg, 3.05 mmol) was added in portions to a mixture of concentrated sulfuric acid (7.0 mL) and 100% nitric acid (6.0 mL) at 0 °C. The mixture was slowly warmed to room temperature and stirred for 12 h. Crushed ice was then added, and the resulting precipitate was filtered, washed with cold water, and air-dried to yield compound **5** in 57% (620 mg) yield as yellow solid.




DSC–TGA (10 °C $min^{-1}$, °C): 154 °C ($T_d$). $^1$H NMR (600 MHz, Acetone–$d_6$): $\delta$ = 9.70 (s, 2H); $^{13}$C NMR (151 MHz, Acetone–$d_6$): $\delta$ = 168.8, 159.6, 143.1 ppm. $^{15}$N NMR (61 MHz, DMSO–$d_6$): 361.8, 335.8, 335.0, 239.7, 226.6 ppm. IR(Neat) $\upsilon_{max}$ 3149, 3093, 1628, 1606, 1526, 1417, 1387, 1343, 1311, 1276, 1220, 1100, 1076, 951, 924, 889, 837, 794, 749, 674, 628, 564, 505, 469 $cm^{-1}$. HRMS (ESI) for $C_7H_2N_9O_6^-$ $(M–HNO_2)^-$: calcd 308.0128, found 308.0117.

**X-ray Crystallography**[7]

Single crystal X-ray data for the compounds **5** was collected using the 'Bruker D8 VENTURE Photon III detector' system [Mo-Kα fine focus sealed tube λ = 0.71073 Å] at 295 K graphite monochromator with a ω scan. Data reduction was performed using Bruker SAINT[2] software. Intensities for absorption were corrected using SADABS 2014/5, Structure solution and refinement were carried out using Bruker SHELX-TL. All non-hydrogen atoms were refined anisotropically. Thermal ellipsoid plot of compound **5** with 50% probability and hydrogen atoms are labelled for clarity shown in Fig. S1.

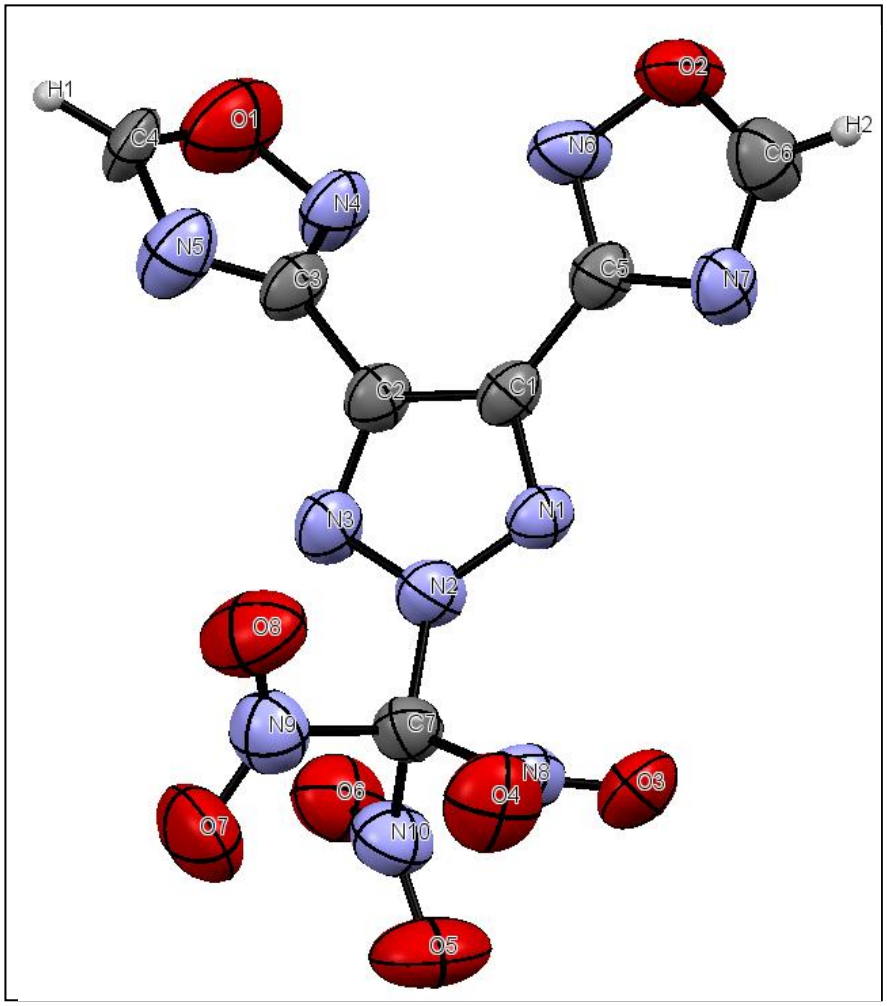



**Figure S1.** Thermal ellipsoid plot of compound **5** with 50% probability and hydrogen atoms are labelled for clarity.

**Table S1** Crystallographic data for compound **5**

| **Compound** | **5** |
|---|---|
| CCDC | 2191899 |
| Formula | $C_7H_2N_{10}O_8$ |
| $M_w$ | 354.19 |
| Crystal system | Monoclinic |
| Space group | $P_{21}$ |
| $T$ [K] | 295 K |
| $a$ [Å] | 8.5672 (4) |
| $b$ [Å] | 8.6047 (3) |
| $c$ [Å] | 9.6790 (4) |
| $\alpha$ [°] | 90 |
| $\beta$ [°] | 108.030 (1) |
| $\gamma$ [°] | 90 |
| Z | 2 |
| V [Å] | 678.48 (5) |
| $D_{calc}$ [g/cm$^3$] | 1.734 |
| μ [mm$^{-1}$] | 0.159 |
| Total reflns | 3394 |
| Unique reflns | 2993 |
| Observed reflns | 2388 |
| $R_1[I > 2\sigma(I)]$ | 0.0751 |
| $wR_2$ [all] | 0.2313 |
| GOF | 1.056 |
| Diffractometer | Bruker D8 VENTURE<br>Photon III detector |

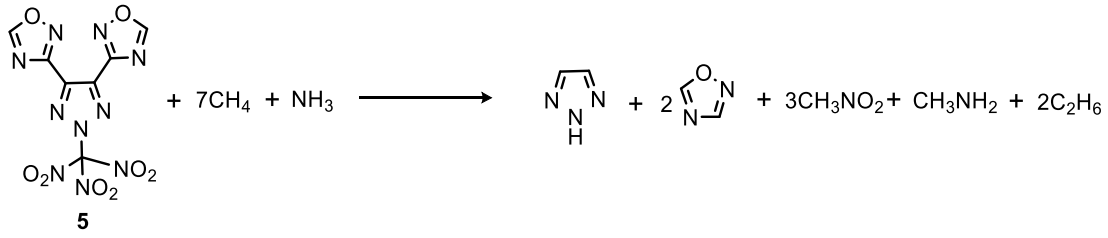
## Hirshfeld Surface Analysis[8]

The Hirshfeld surface image (Fig. 4, in manuscript) in which, the red spots signify the high contact populations, while blue and white spots are for low contact populations. This suggests that the negative (red) or positive value (blue and white) of $d_{norm}$ depends on the intermolecular contacts being shorter (red) or longer (blue and white) than the van der Waals separations. For each point on the Hirshfeld surface, the normalized contact distance ($d_{norm}$) was determined by the equation shown below.

$$[d_{norm} = ( d_i - d_i^{vdW})/r_i^{vdW} + (d_e - d_e^{vdW}/r_e^{vdW}]$$

In which $d_i$ is measured from the surface of nearest atom interior to the surface interior, while $d_e$ is measured from the surface of nearest atom exterior to the surface interior, where $r_i^{vdW}$ and $r_e^{vdW}$ are the van der Waals radii of the atoms. Hirshfeld surface graphs and two-dimensional fingerprint plots of **5** were analyzed using crystal explorer 17.5 software.

## Isodesmic reactions for the prediction of heat of formation[9]




**5**

## References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D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

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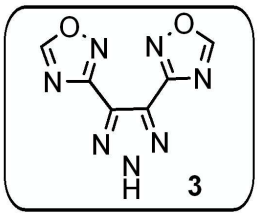





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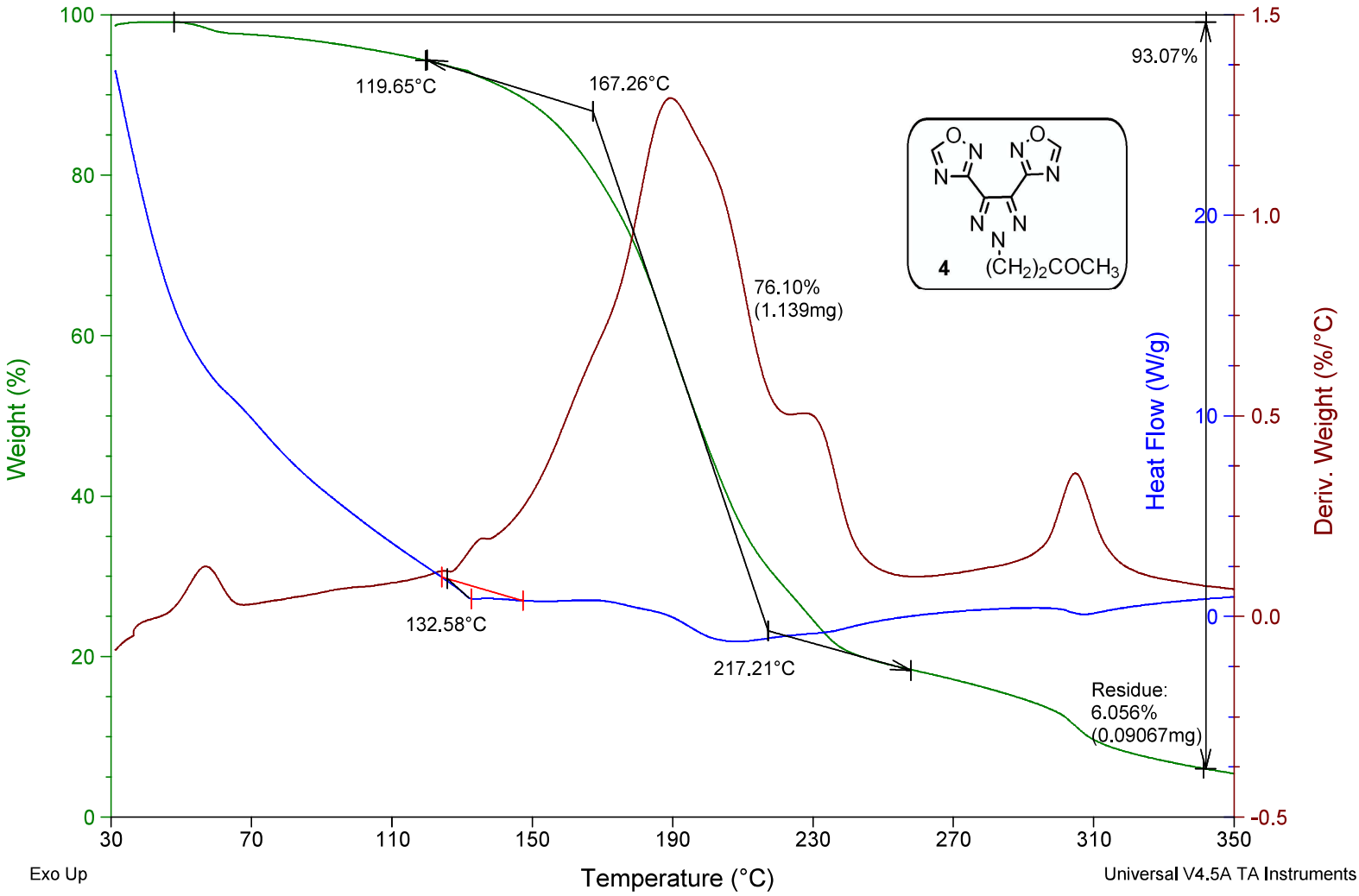

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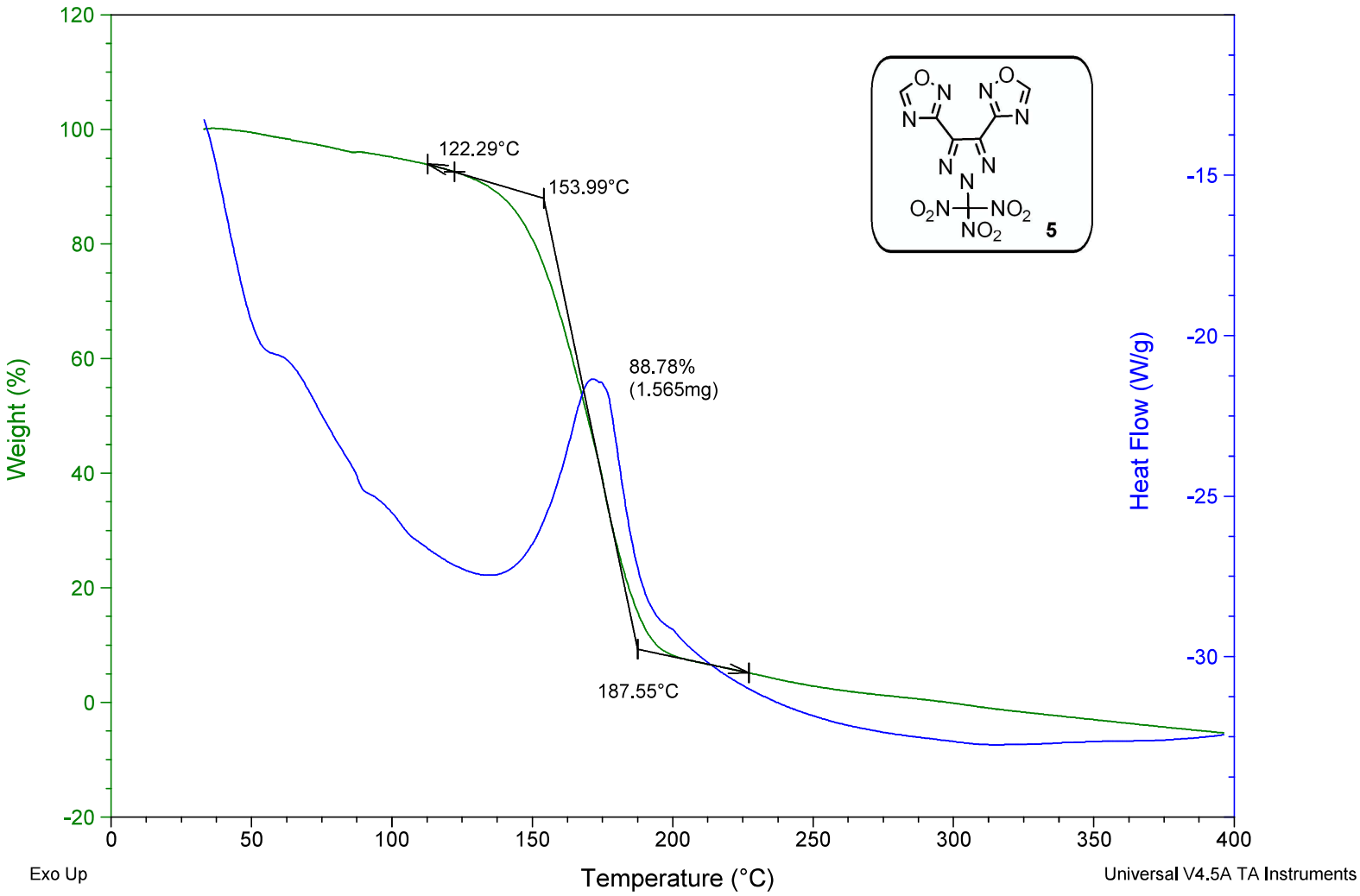

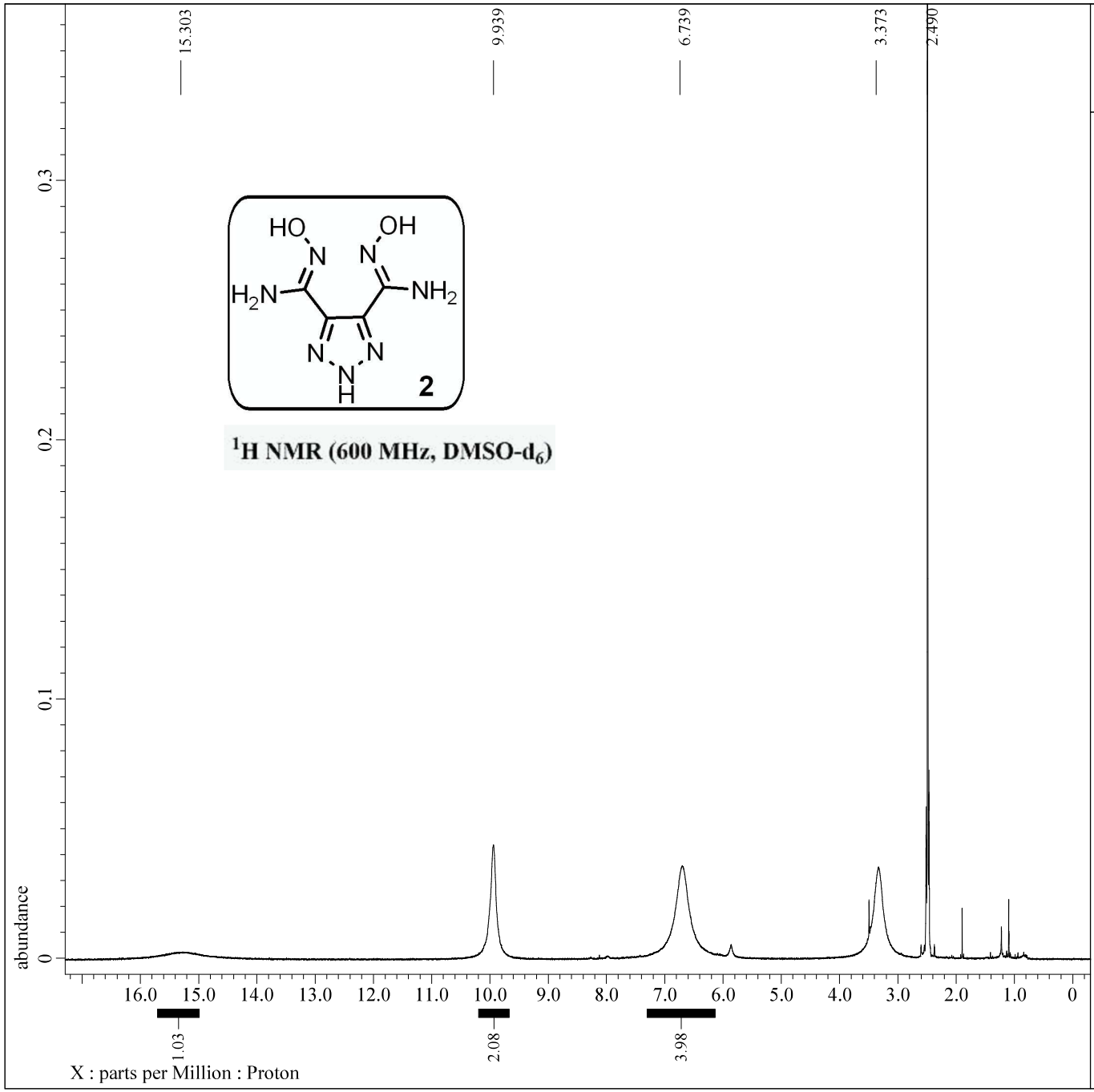


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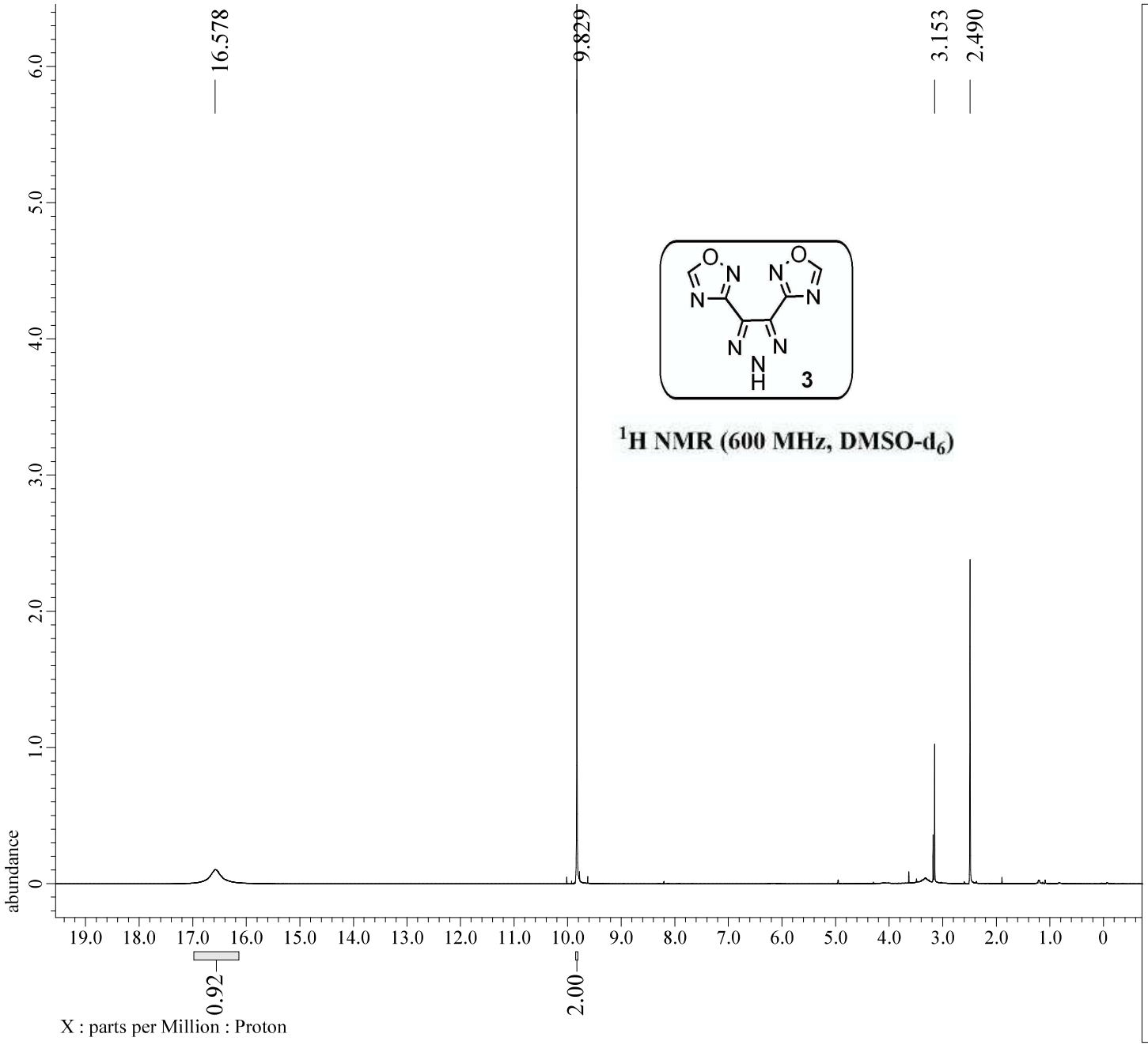


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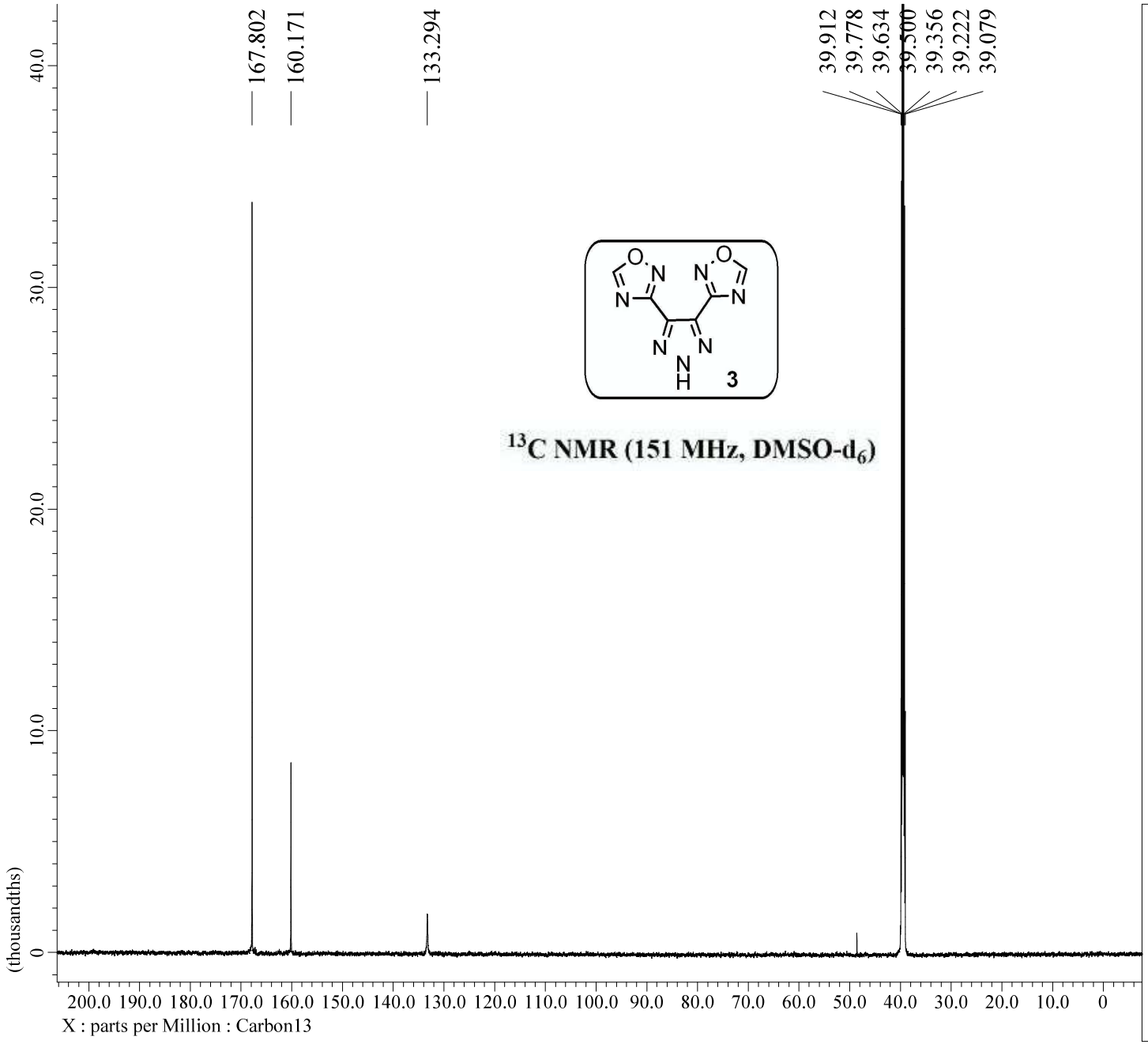


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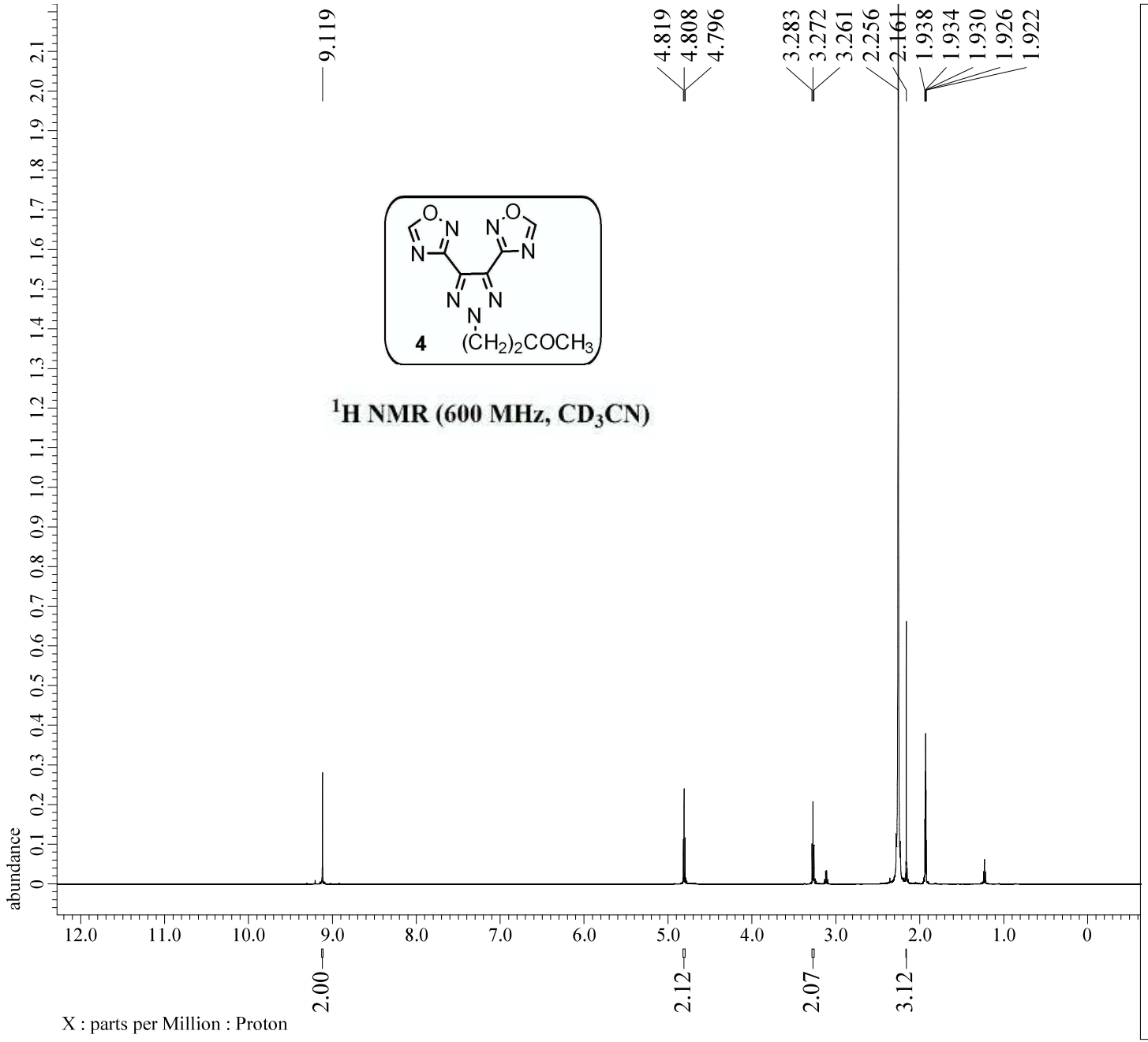
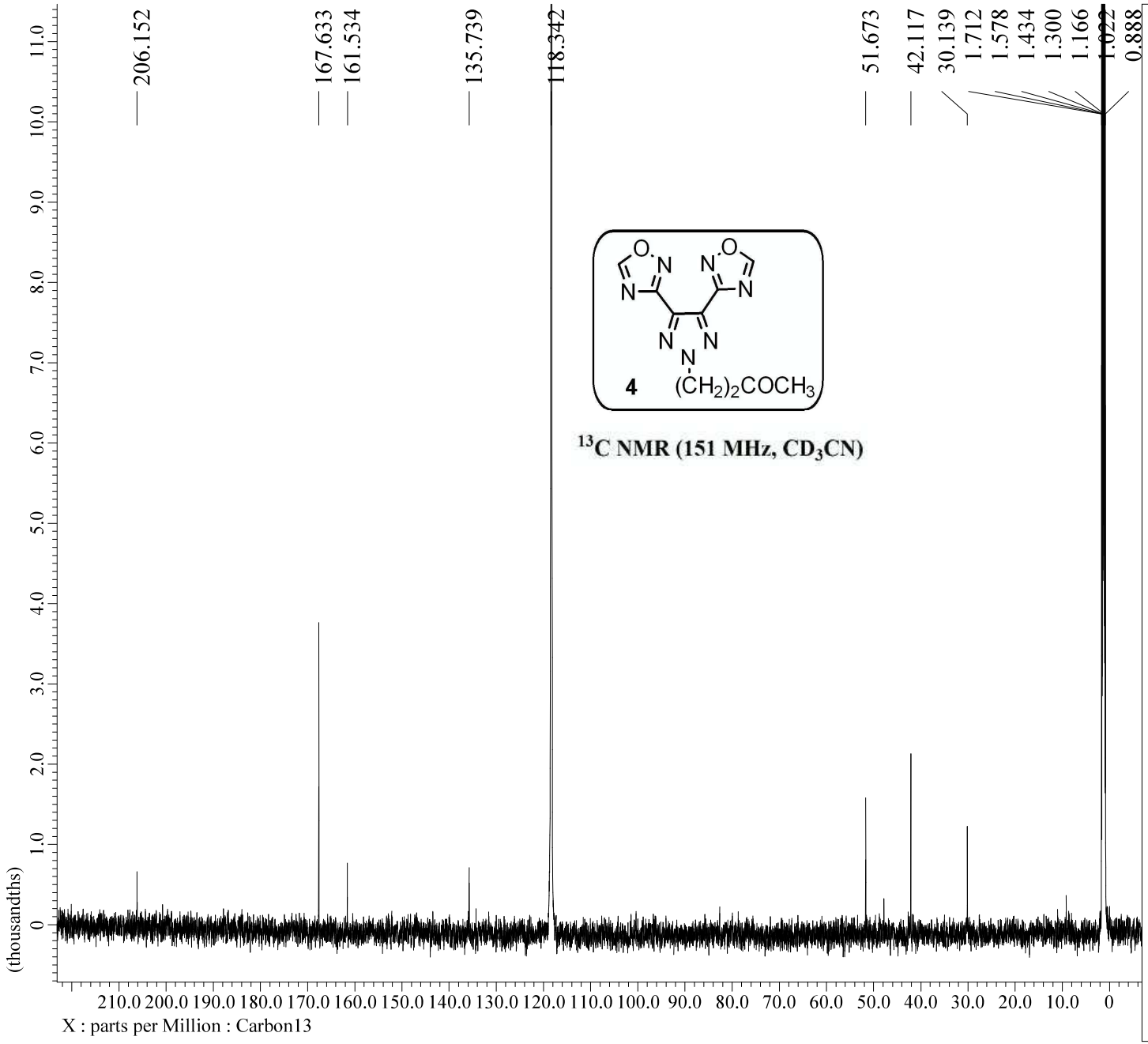
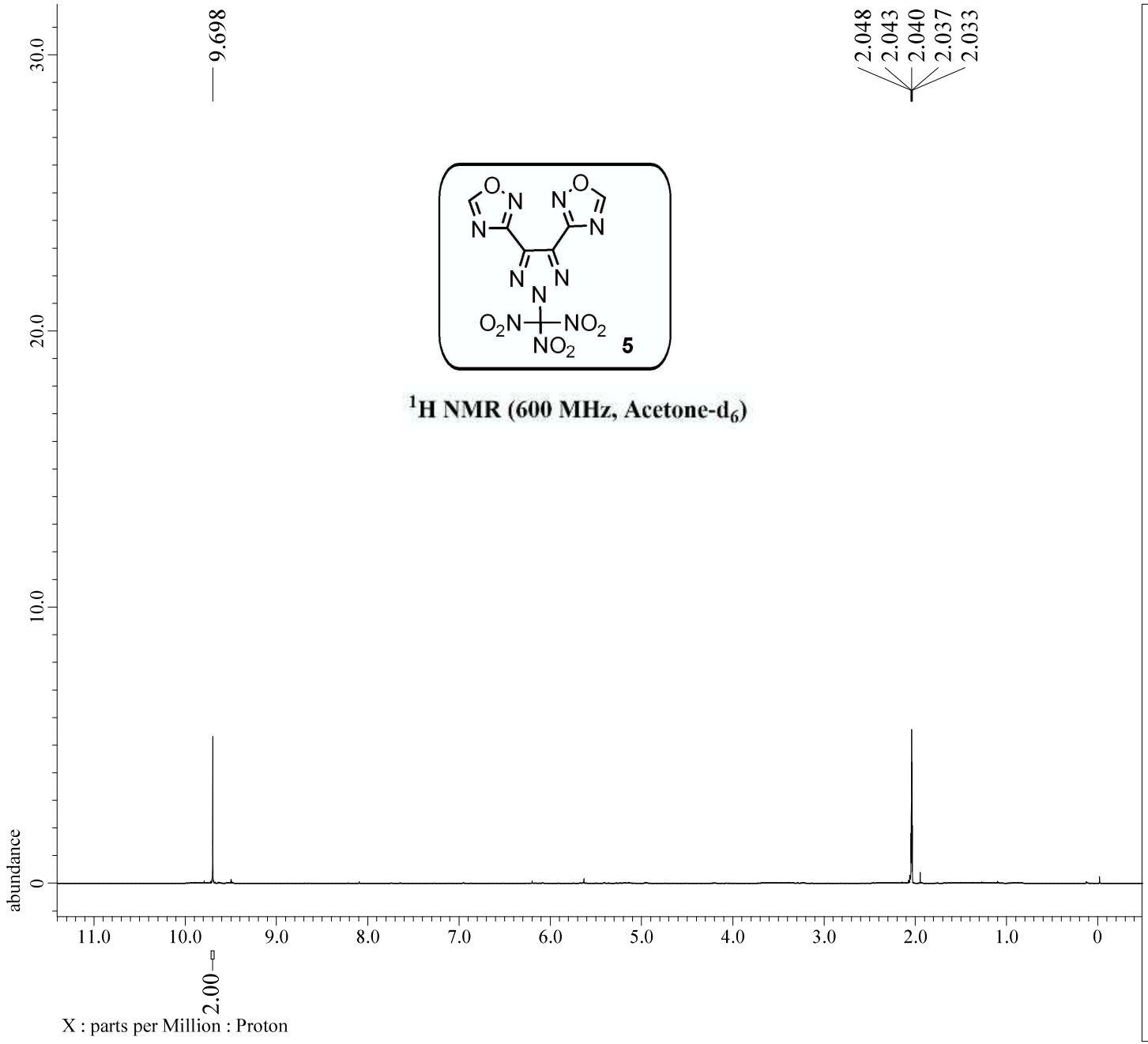
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = ACRHEM_UOH |
| Spectrometer | = JNM-ECZ600R/M1 |
| Field_Strength | = 14.09636928[T] (60 |
| X_Acq_Duration | = 0.34603008[s] |
| X_Domain | = Carbon13 |
| X_Freq | = 150.91343039[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 4 |
| X_Resolution | = 2.88992217[Hz] |
| X_Sweep | = 47.34848485[kHz] |
| X_Sweep_Clipped | = 37.87878788[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 600.1723046[MHz] |
| Irr_Offset | = 5[ppm] |
| Blanking | = 2[us] |
| Clipped | = FALSE |
| Scans | = 2048 |
| Total_Scans | = 2048 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 19.7[dC] |
| X_90_Width | = 11[us] |
| X_Acq_Time | = 0.34603008[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 10.3[dB] |
| X_Pulse | = 3.66666667[us] |
| Irr_Atn_Dec | = 33.452[dB] |
| Irr_Atn_Dec_Calc | = 33.452[dB] |
| Irr_Atn_Dec_Default_Calc | = 33.452[dB] |
| Irr_Atn_Noe | = 33.452[dB] |
| Irr_Dec_Bandwidth_Hz | = 7.23684211[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 12.05794078[ppm] |
| Irr_Dec_Freq | = 600.1723046[MHz] |
| Irr_Dec_Merit_Factor | = 2.2 |
| Irr_Decoupling | = TRUE |
| Irr_Noe | = TRUE |
| Irr_Noise | = WALTZ |
| Irr_Offset_Default | = 5[ppm] |
| Irr_Pwidth | = 76[us] |
| Irr_Pwidth_Default | = 76[us] |
| Irr_Pwidth_Default_Calc | = 76[us] |
| Irr_Pwidth_Temp1 | = 76[us] |
| Irr_Wurst | = FALSE |
| Decimation_Rate | = 0 |
| Experiment_Path | = c:\Program Files\J |
| Initial_Wait | = 1[s] |
| Noe_Time | = 2[s] |
| Noe_Time_Flag | = FALSE |
| Relaxation_Delay_Calc | = 0[s] |
| Relaxation_Delay_Temp | = 2[s] |




```
Filename                = Vs-6-45b_Proton-1-2.j
Author                  = delta
Experiment              = proton_auto.jxp
Sample_Id               = Vs-6-45b
Solvent                 = ACETONITRILE-D3
Actual_Start_Time       = 15-DEC-2021 17:13:18
Revision_Time           = 17-DEC-2021 03:15:59

Comment                 = single_pulse
Data_Format             = 1D COMPLEX
Dim_Size                = 52429
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Site                    = ACRHEM_UOH
Spectrometer            = JNM-ECZ600R/M1

Field_Strength          = 14.09636928[T] (600[M
X_Acq_Duration          = 0.72876032[s]
X_Domain                = Proton
X_Freq                  = 600.1723046[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 1.37219326[Hz]
X_Sweep                 = 22.48201439[kHz]
X_Sweep_Clipped         = 17.98561151[kHz]
Irr_Domain              = Proton
Irr_Freq                = 600.1723046[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 600.1723046[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 8
Total_Scans             = 8

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 20.9[dC]
X_90_Width              = 6.89[us]
X_Acq_Time              = 0.72876032[s]
X_Angle                 = 45[deg]
X_Atn                   = 12.6[dB]
X_Pulse                 = 3.445[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Experiment_Path         = c:\Program Files\JEOL
Initial_Wait            = 1[s]
Phase                   = {0, 90, 270, 180, 180
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 5.72876032[s]
```




| | |
|---|---|
| Filename | = Vs-6-45b_Carbon-1- |
| Author | = delta |
| Experiment | = carbon_auto.jxp |
| Sample_Id | = Vs-6-45b |
| Solvent | = ACETONITRILE-D3 |
| Actual_Start_Time | = 15-DEC-2021 17:14: |
| Revision_Time | = 17-DEC-2021 03:04: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| X_Domain | = Carbon13 |
| Dim_Title | = Carbon13 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Site | = ACRHEM_UOH |
| Spectrometer | = JNM-ECZ600R/M1 |
| Field_Strength | = 14.09636928[T] (60 |
| X_Acq_Duration | = 0.34603008[s] |
| X_Domain | = Carbon13 |
| X_Freq | = 150.91343039[MHz] |
| X_Offset | = 100[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 4 |
| X_Resolution | = 2.88992217[Hz] |
| X_Sweep | = 47.34848485[kHz] |
| X_Sweep_Clipped | = 37.87878788[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 600.1723046[MHz] |
| Irr_Offset | = 5[ppm] |
| Blanking | = 2[us] |
| Clipped | = FALSE |
| Scans | = 545 |
| Total_Scans | = 545 |
| Relaxation_Delay | = 2[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 21[dC] |
| X_90_Width | = 11[us] |
| X_Acq_Time | = 0.34603008[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 10.3[dB] |
| X_Pulse | = 3.66666667[us] |
| Irr_Atn_Dec | = 33.452[dB] |
| Irr_Atn_Dec_Calc | = 33.452[dB] |
| Irr_Atn_Dec_Default_Calc | = 33.452[dB] |
| Irr_Atn_Noe | = 33.452[dB] |
| Irr_Dec_Bandwidth_Hz | = 7.23684211[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 12.05794078[ppm] |
| Irr_Dec_Freq | = 600.1723046[MHz] |
| Irr_Dec_Merit_Factor | = 2.2 |
| Irr_Decoupling | = TRUE |
| Irr_Noe | = TRUE |
| Irr_Noise | = WALTZ |
| Irr_Offset_Default | = 5[ppm] |
| Irr_Pwidth | = 76[us] |
| Irr_Pwidth_Default | = 76[us] |
| Irr_Pwidth_Default_Calc | = 76[us] |
| Irr_Pwidth_Temp1 | = 76[us] |
| Irr_Wurst | = FALSE |
| Decimation_Rate | = 0 |
| Experiment_Path | = c:\Program Files\J |
| Initial_Wait | = 1[s] |
| Noe_Time | = 2[s] |
| Noe_Time_Flag | = FALSE |
| Relaxation_Delay_Calc | = 0[s] |
| Relaxation_Delay_Temp | = 2[s] |

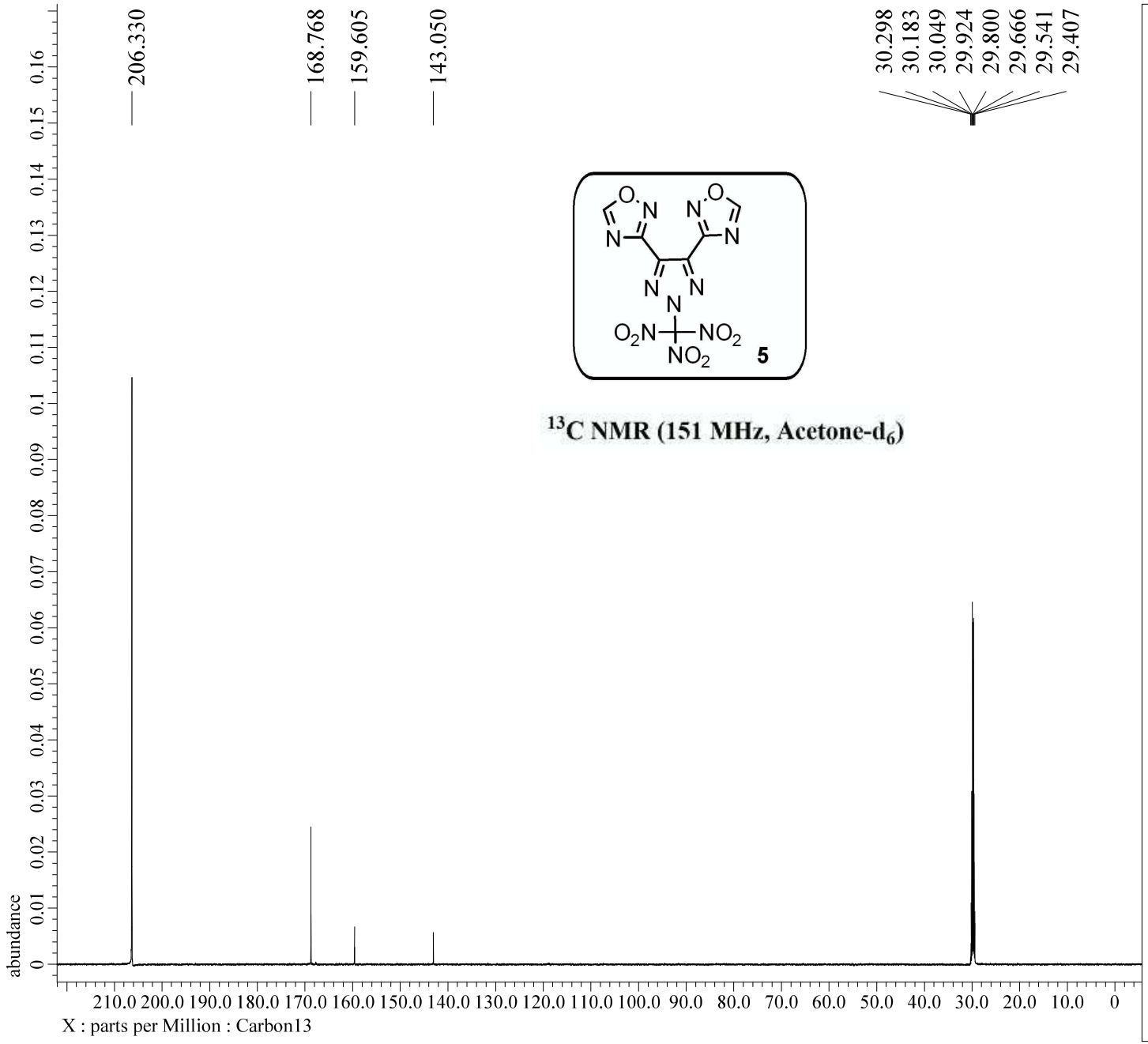






**$^1$H NMR (600 MHz, Acetone-d$_6$)**

| | |
|---|---|
| Filename | = VS-7-6B 1_Proton-1-1 |
| Author | = delta |
| Experiment | = proton_auto.jxp |
| Sample_Id | = VS-7-6B 1 |
| Solvent | = ACETONE-D6 |
| Actual_Start_Time | = 15-JUL-2020 11:16:58 |
| Revision_Time | = 24-JUL-2021 19:45:40 |
| Comment | = single_pulse |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 13107 |
| X_Domain | = Proton |
| Dim_Title | = Proton |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ600R/M1 |
| Field_Strength | = 14.09636928[T] (600[M |
| X_Acq_Duration | = 1.45227776[s] |
| X_Domain | = Proton |
| X_Freq | = 600.1723046[MHz] |
| X_Offset | = 5[ppm] |
| X_Points | = 16384 |
| X_Prescans | = 1 |
| X_Resolution | = 0.68857351[Hz] |
| X_Sweep | = 11.28158845[kHz] |
| X_Sweep_Clipped | = 9.02527076[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 600.1723046[MHz] |
| Irr_Offset | = 5[ppm] |
| Tri_Domain | = Proton |
| Tri_Freq | = 600.1723046[MHz] |
| Tri_Offset | = 5[ppm] |
| Blanking | = 2[us] |
| Clipped | = FALSE |
| Scans | = 16 |
| Total_Scans | = 16 |
| Relaxation_Delay | = 5[s] |
| Recvr_Gain | = 46 |
| Temp_Get | = 21.3[dC] |
| X_90_Width | = 6.89[us] |
| X_Acq_Time | = 1.45227776[s] |
| X_Angle | = 45[deg] |
| X_Atn | = 12.6[dB] |
| X_Pulse | = 3.445[us] |
| Irr_Mode | = Off |
| Tri_Mode | = Off |
| Dante_Loop | = 500 |
| Dante_Presat | = FALSE |
| Decimation_Rate | = 0 |
| Experiment_Path | = c:\Program Files\JEOL |
| Initial_Wait | = 1[s] |
| Phase | = {0, 90, 270, 180, 180 |
| Presat_Time | = 5[s] |
| Presat_Time_Flag | = FALSE |
| Relaxation_Delay_Calc | = 0[s] |
| Relaxation_Delay_Temp | = 5[s] |
| Repetition_Time | = 6.45227776[s] |

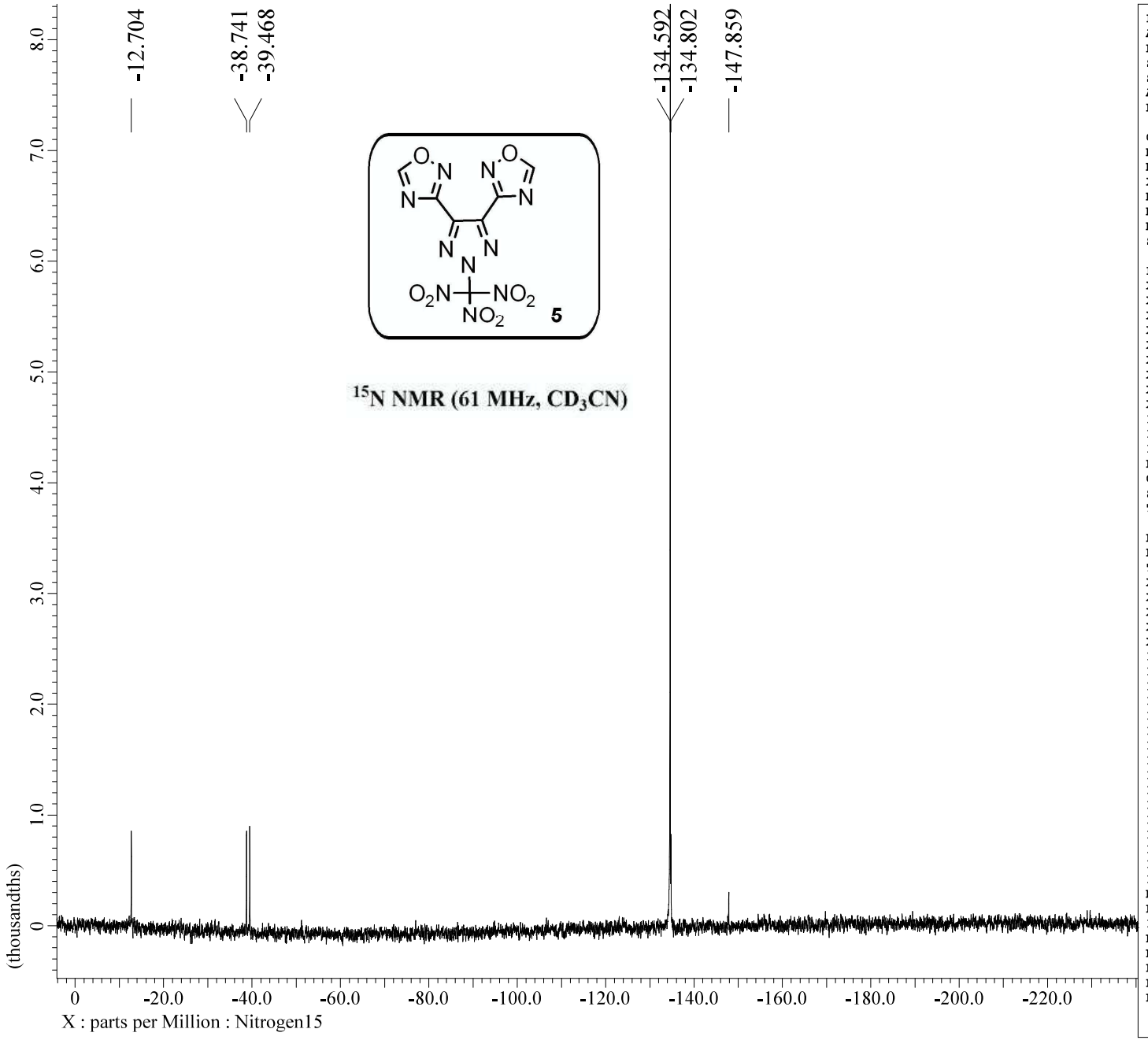






**$^{13}$C NMR (151 MHz, Acetone-d$_6$)**

```
Filename                    = VS-7-6B 1_Carbon-2
Author                      = delta
Experiment                  = carbon_auto.jxp
Sample_Id                   = VS-7-6B 1
Solvent                     = ACETONE-D6
Actual_Start_Time           = 15-JUL-2020 11:19:
Revision_Time               = 24-JUL-2021 19:48:

Comment                     = single pulse decou
Data_Format                 = 1D COMPLEX
Dim_Size                    = 26214
X_Domain                    = Carbon13
Dim_Title                   = Carbon13
Dim_Units                   = [ppm]
Dimensions                  = X
Spectrometer                = JNM-ECZ600R/M1

Field_Strength              = 14.09636928[T] (60
X_Acq_Duration              = 0.69206016[s]
X_Domain                    = Carbon13
X_Freq                      = 150.91343039[MHz]
X_Offset                    = 100[ppm]
X_Points                    = 32768
X_Prescans                  = 4
X_Resolution                = 1.44496109[Hz]
X_Sweep                     = 47.34848485[kHz]
X_Sweep_Clipped             = 37.87878788[kHz]
Irr_Domain                  = Proton
Irr_Freq                    = 600.1723046[MHz]
Irr_Offset                  = 5[ppm]
Blanking                    = 2[us]
Clipped                     = FALSE
Scans                       = 413
Total_Scans                 = 413

Relaxation_Delay            = 2[s]
Recvr_Gain                  = 50
Temp_Get                    = 21.3[dC]
X_90_Width                  = 11[us]
X_Acq_Time                  = 0.69206016[s]
X_Angle                     = 30[deg]
X_Atn                       = 10.3[dB]
X_Pulse                     = 3.66666667[us]
Irr_Atn_Dec                 = 33.452[dB]
Irr_Atn_Dec_Calc            = 33.452[dB]
Irr_Atn_Dec_Default_Calc    = 33.452[dB]
Irr_Atn_Noe                 = 33.452[dB]
Irr_Dec_Bandwidth_Hz        = 7.23684211[kHz]
Irr_Dec_Bandwidth_Ppm       = 12.05794078[ppm]
Irr_Dec_Freq                = 600.1723046[MHz]
Irr_Dec_Merit_Factor        = 2.2
Irr_Decoupling              = TRUE
Irr_Noe                     = TRUE
Irr_Noise                   = WALTZ
Irr_Offset_Default          = 5[ppm]
Irr_Pwidth                  = 76[us]
Irr_Pwidth_Default          = 76[us]
Irr_Pwidth_Default_Calc     = 76[us]
Irr_Pwidth_Temp1            = 76[us]
Irr_Wurst                   = FALSE
Decimation_Rate             = 0
Experiment_Path             = c:\Program Files\J
Initial_Wait                = 1[s]
Noe_Time                    = 2[s]
Noe_Time_Flag               = FALSE
Relaxation_Delay_Calc       = 0[s]
Relaxation_Delay_Temp       = 2[s]
Repetition_Time             = 2.69206016[s]
```




| | |
|---|---|
| Filename | = VS-7-6b-15N_MBR-NM |
| Author | = delta |
| Experiment | = single_pulse_dec.j |
| Sample_Id | = VS-7-6b-15N |
| Solvent | = ACETONITRILE-D3 |
| Actual_Start_Time | = 22-AUG-2020 18:25: |
| Revision_Time | = 24-FEB-2023 18:17: |
| Comment | = single pulse decou |
| Data_Format | = 1D COMPLEX |
| Dim_Size | = 26214 |
| X_Domain | = Nitrogen15 |
| Dim_Title | = Nitrogen15 |
| Dim_Units | = [ppm] |
| Dimensions | = X |
| Spectrometer | = JNM-ECZ600R/M1 |
| Field_Strength | = 14.09636928[T] (60 |
| X_Acq_Duration | = 0.85983232[s] |
| X_Domain | = Nitrogen15 |
| X_Freq | = 60.81520929[MHz] |
| X_Offset | = 214.12266[ppm] |
| X_Points | = 32768 |
| X_Prescans | = 4 |
| X_Resolution | = 1.45377182[Hz] |
| X_Sweep | = 38.1097561[kHz] |
| X_Sweep_Clipped | = 30.48780488[kHz] |
| Irr_Domain | = Proton |
| Irr_Freq | = 600.1723046[MHz] |
| Irr_Offset | = 5[ppm] |
| Blanking | = 5[us] |
| Clipped | = TRUE |
| Scans | = 9172 |
| Total_Scans | = 9172 |
| Relaxation_Delay | = 15[s] |
| Recvr_Gain | = 56 |
| Temp_Get | = 20.3[dC] |
| X_90_Width | = 24.21[us] |
| X_Acq_Time | = 0.68786586[s] |
| X_Angle | = 30[deg] |
| X_Atn | = 9.9[dB] |
| X_Pulse | = 8.07[us] |
| Irr_Atn_Dec | = 33.452[dB] |
| Irr_Atn_Dec_Calc | = 33.452[dB] |
| Irr_Atn_Dec_Default_Calc | = 33.452[dB] |
| Irr_Dec_Bandwidth_Hz | = 7.23684211[kHz] |
| Irr_Dec_Bandwidth_Ppm | = 12.05794078[ppm] |
| Irr_Dec_Freq | = 600.1723046[MHz] |
| Irr_Dec_Merit_Factor | = 2.2 |
| Irr_Decoupling | = TRUE |
| Irr_Noe | = FALSE |
| Irr_Noise | = WALTZ |
| Irr_Offset_Default | = 5[ppm] |
| Irr_Pwidth | = 76[us] |
| Irr_Pwidth_Default | = 76[us] |
| Irr_Pwidth_Default_Calc | = 76[us] |
| Irr_Pwidth_Temp1 | = 76[us] |
| Irr_Wurst | = FALSE |
| Decimation_Rate | = 0 |
| Experiment_Path | = C:\Users\delta\Doc |
| Initial_Wait | = 1[s] |
| Noe_Time | = 15[s] |
| Noe_Time_Flag | = FALSE |
| Relaxation_Delay_Calc | = 0[s] |
| Relaxation_Delay_Temp | = 15[s] |
| Repetition_Time | = 15.68786586[s] |