*New J. Chem. 2020 · ISSN*

# Electronic Supplementary Information (ESI)

# *Energetic N-azidomethyl derivatives of polynitro hexaazaisowurtzitanes series: the most highly enthalpy analogues of CL-20*

Oleg A. Luk′yanov, Vladimir V. Parakhin, Nina I. Shlykova, Artem O. Dmitrienko, Elizaveta K. Melnikova, Tatiana S. Kon′kova, Konstantin A. Monogarov and Dmitry B. Meerov

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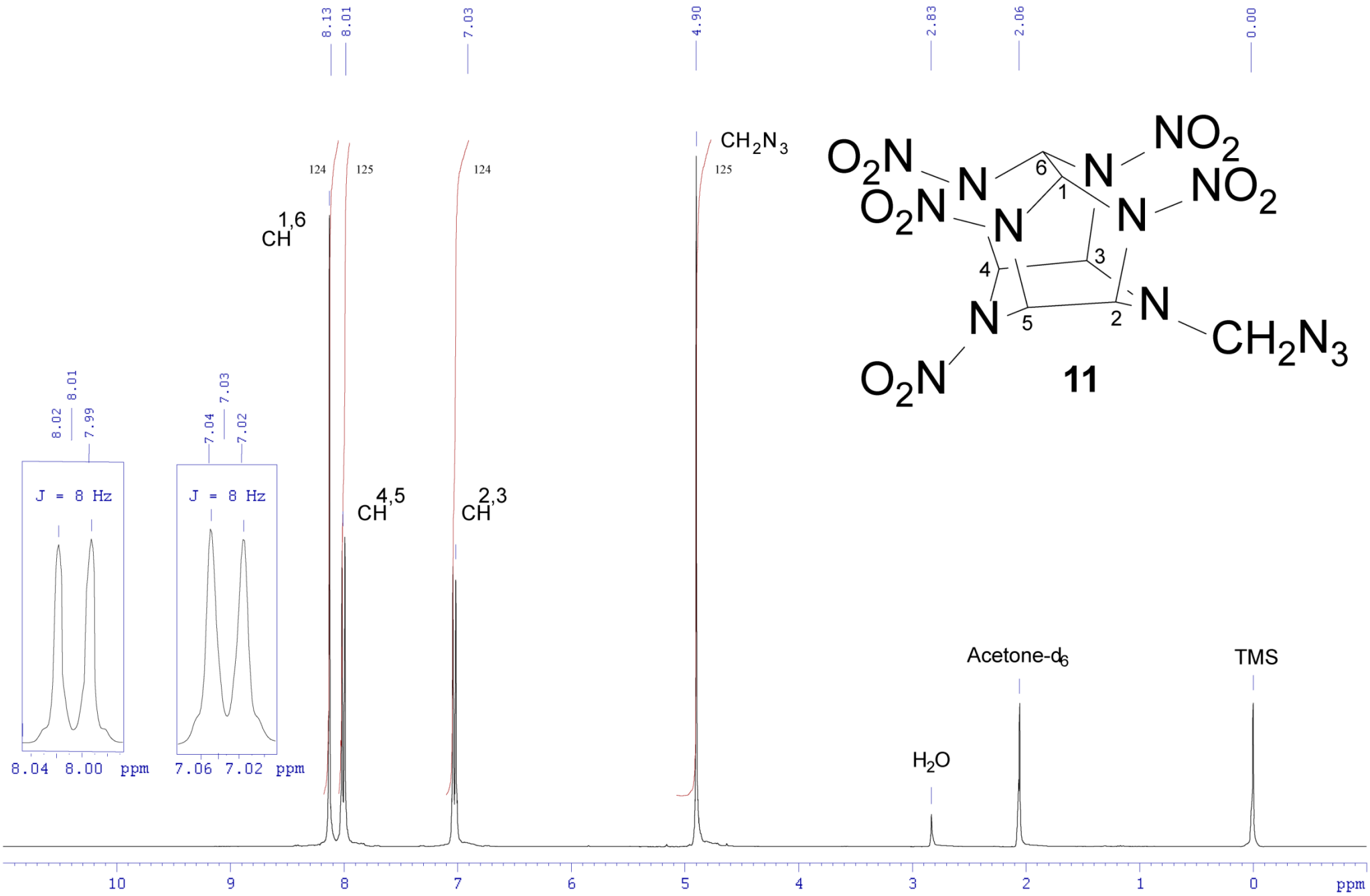
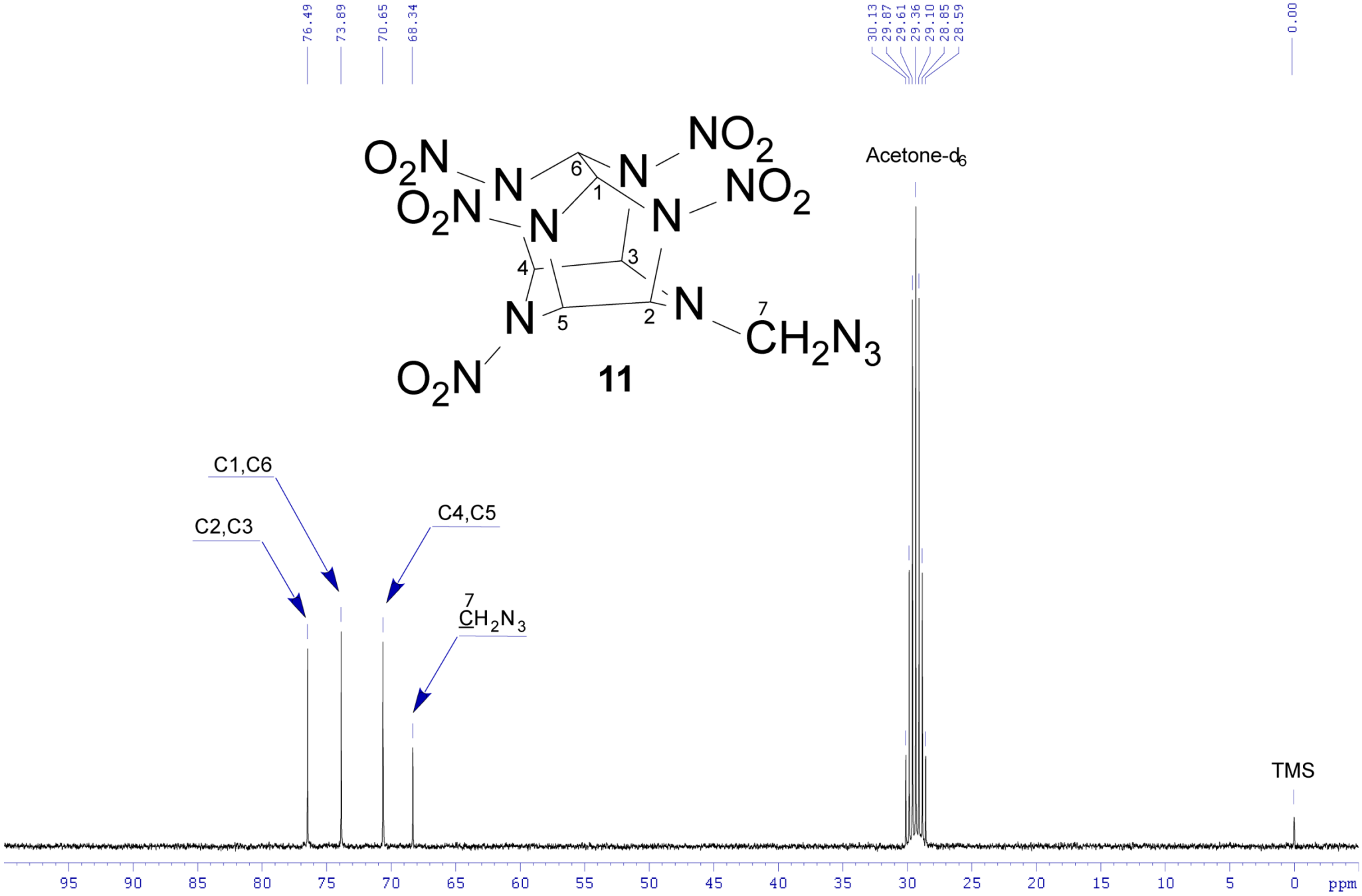
# $^1$H NMR (300.1 MHz, [D$_6$]acetone) spectrum of compound 11

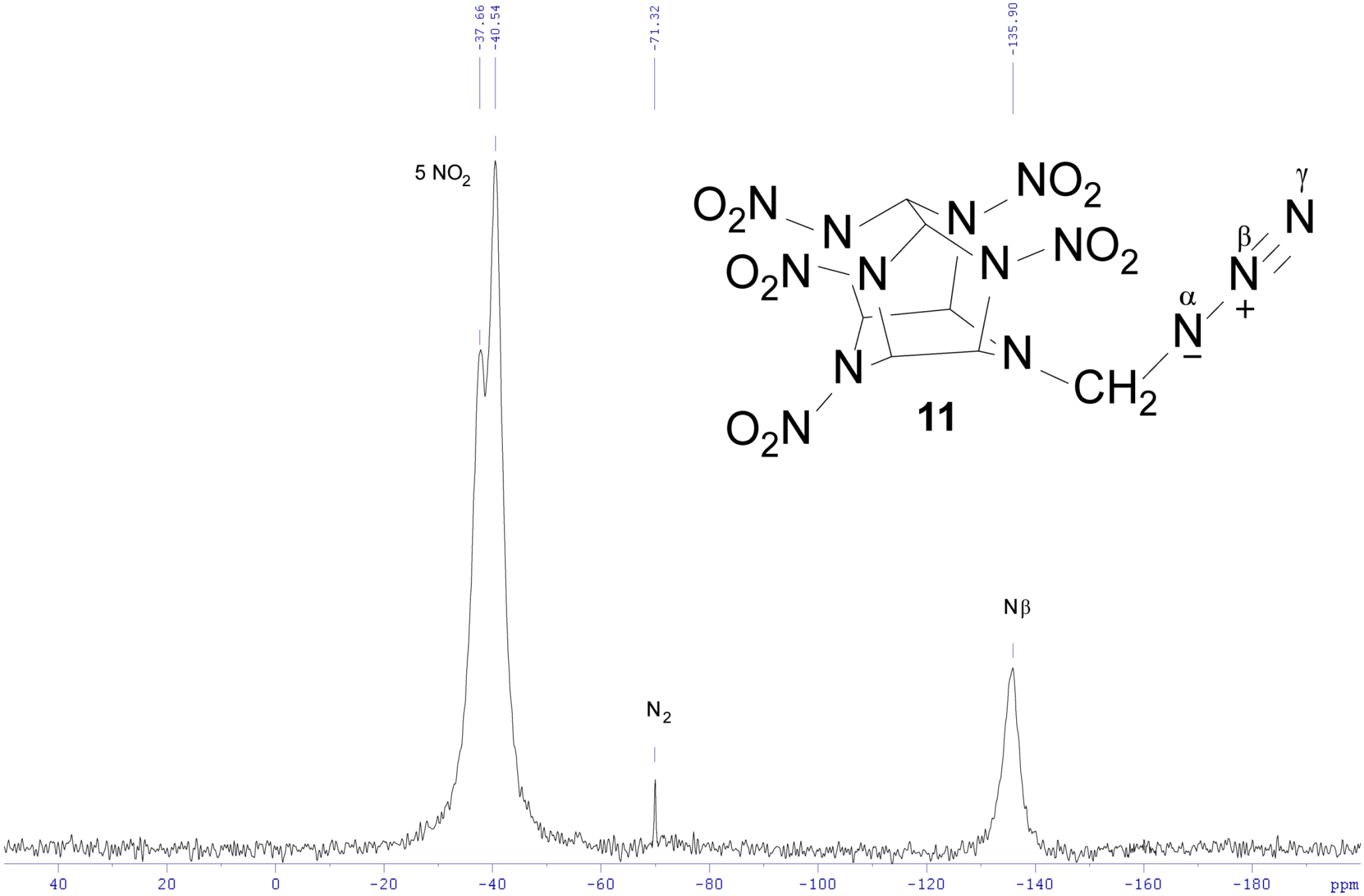


# $^{13}$C NMR (75.5 MHz, [D$_6$]acetone) spectrum of compound 11

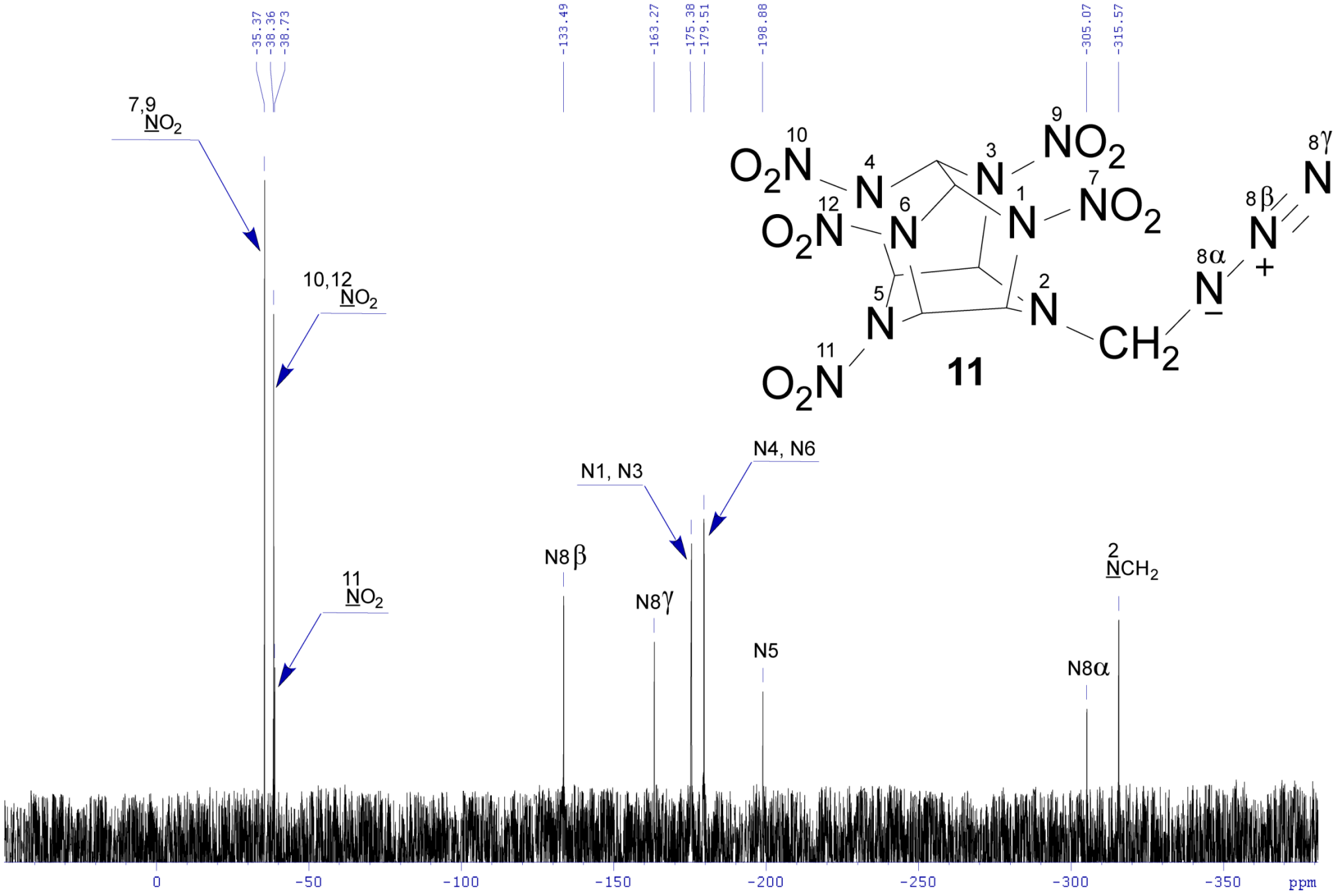



11

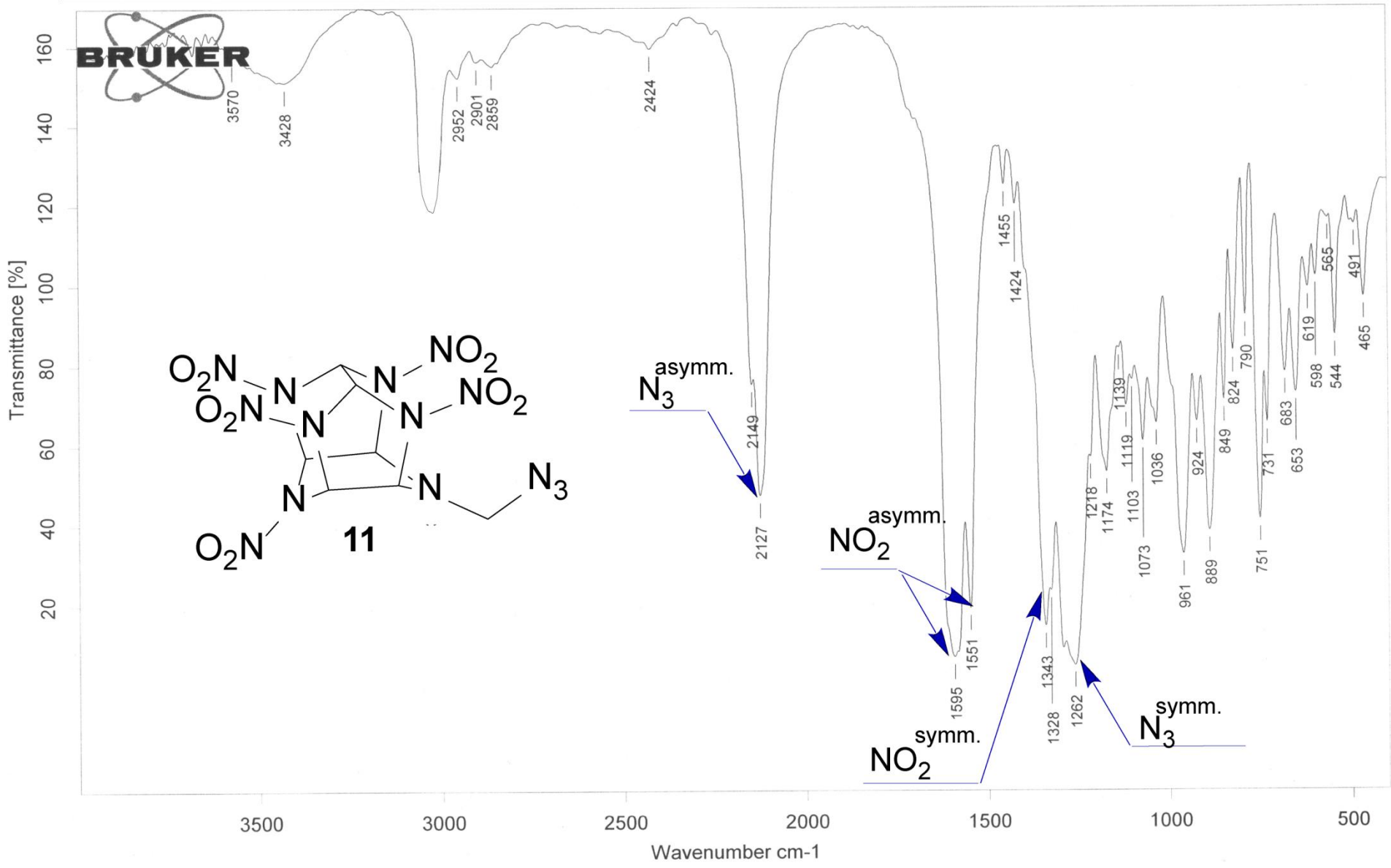
## $^{14}$N NMR (21.7 MHz, [$D_6$]acetone) spectrum of compound 11



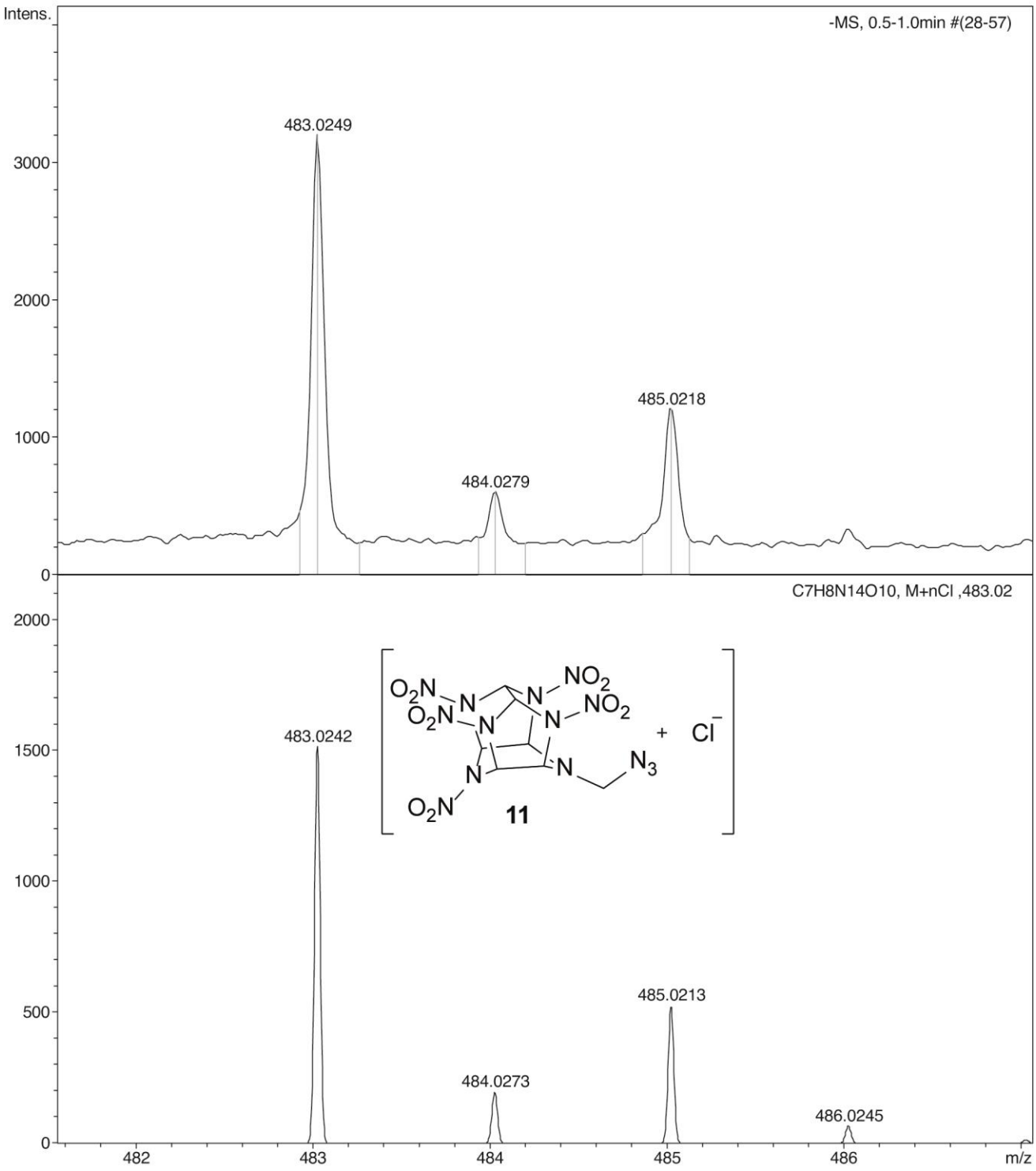
**$^{15}$N NMR ([INVGATED],30.4 MHz,[$D_6$]acetone) spectrum of compound 11**



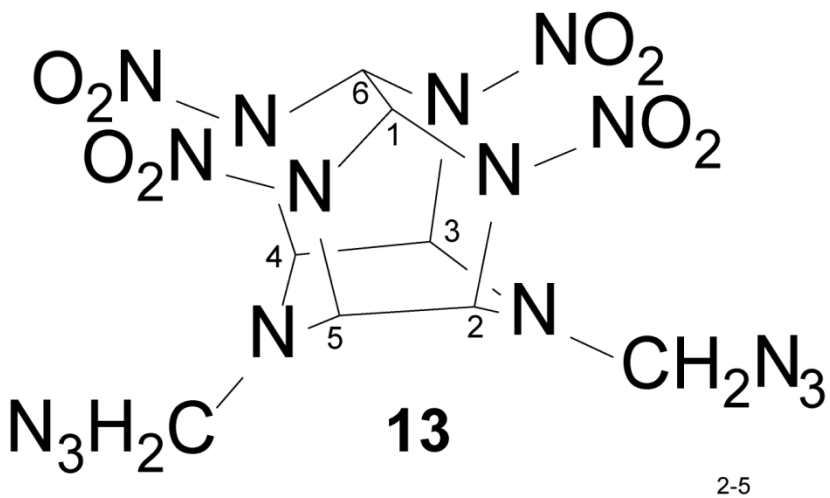
# IR (KBr) spectrum of compound 11



# HRMS (ESI) for compound 11

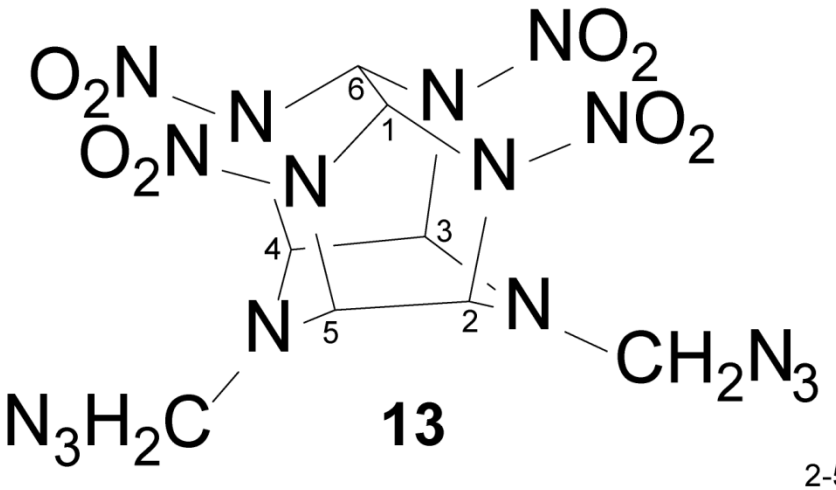


# $^1$H NMR (300.1 MHz, [D$_6$]acetone) spectrum of compound 13



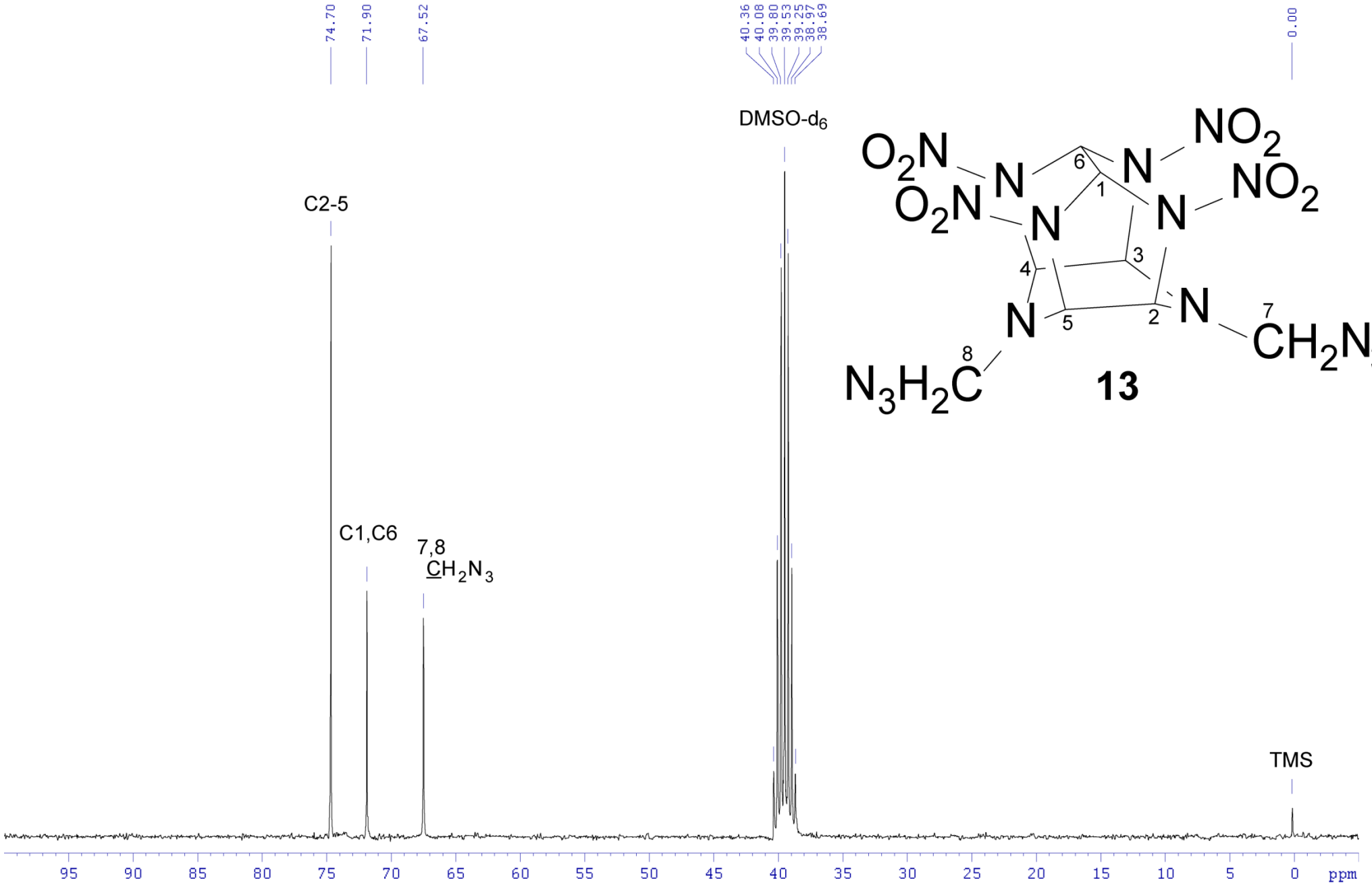

**13**

# $^1$H NMR (300.1 MHz, [D$_6$]DMSO) spectrum of compound 13




**13**

## $^{13}$C NMR (75.5 MHz, [D$_6$]DMSO) spectrum of compound 13

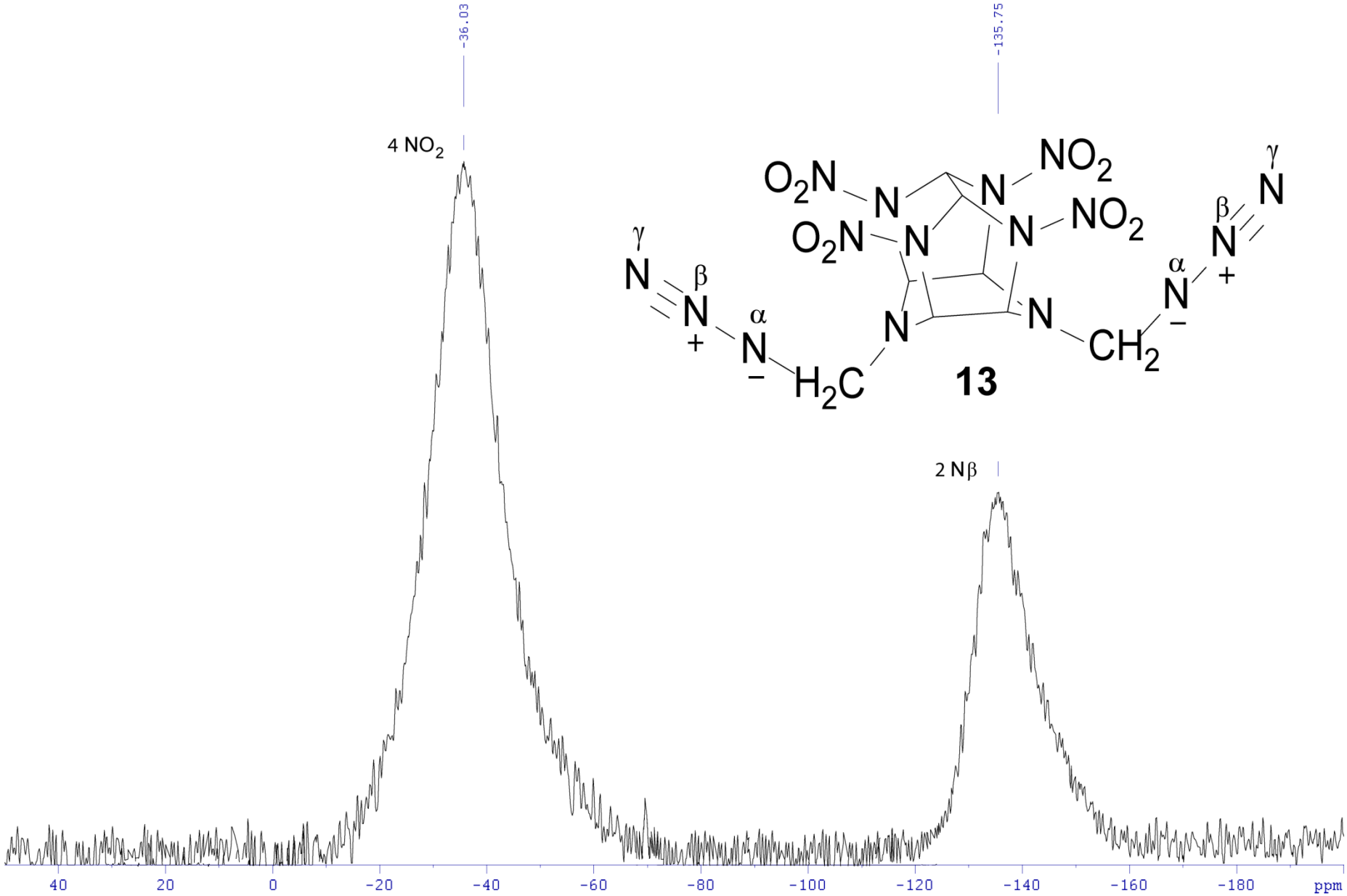






**13**

**$^{14}$N NMR (21.7 MHz, [D$_6$]DMSO) spectrum of compound 13**

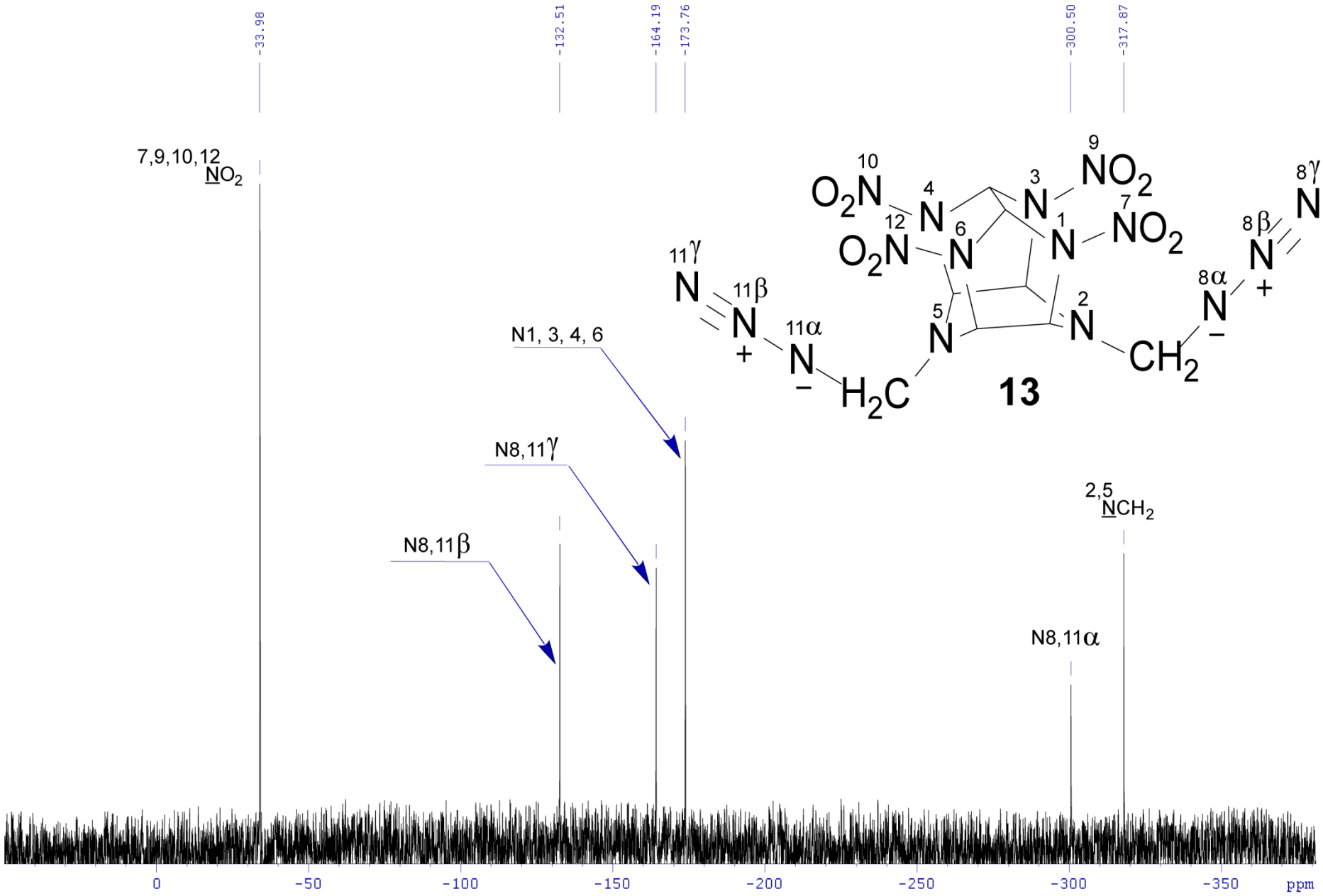




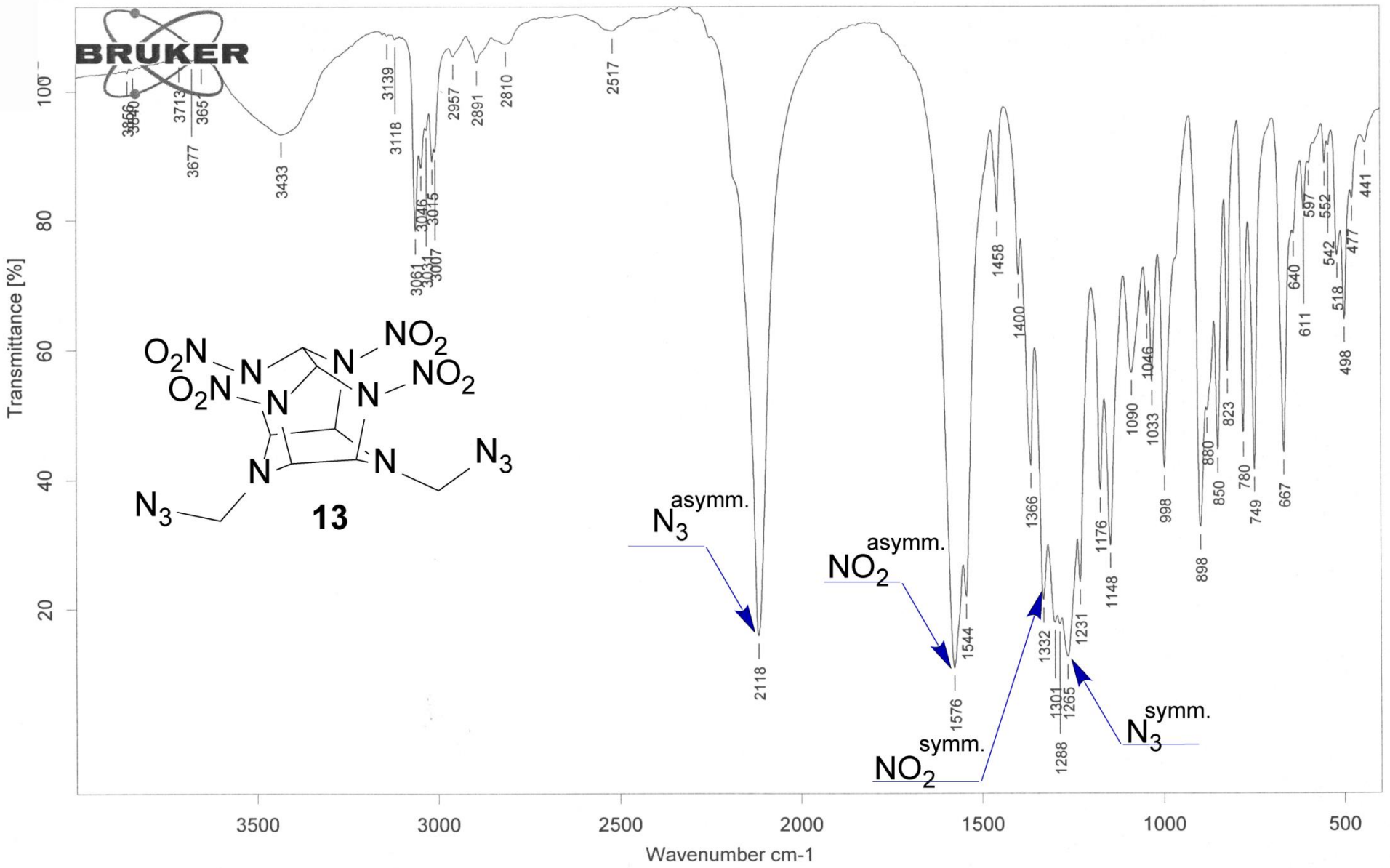


**13**

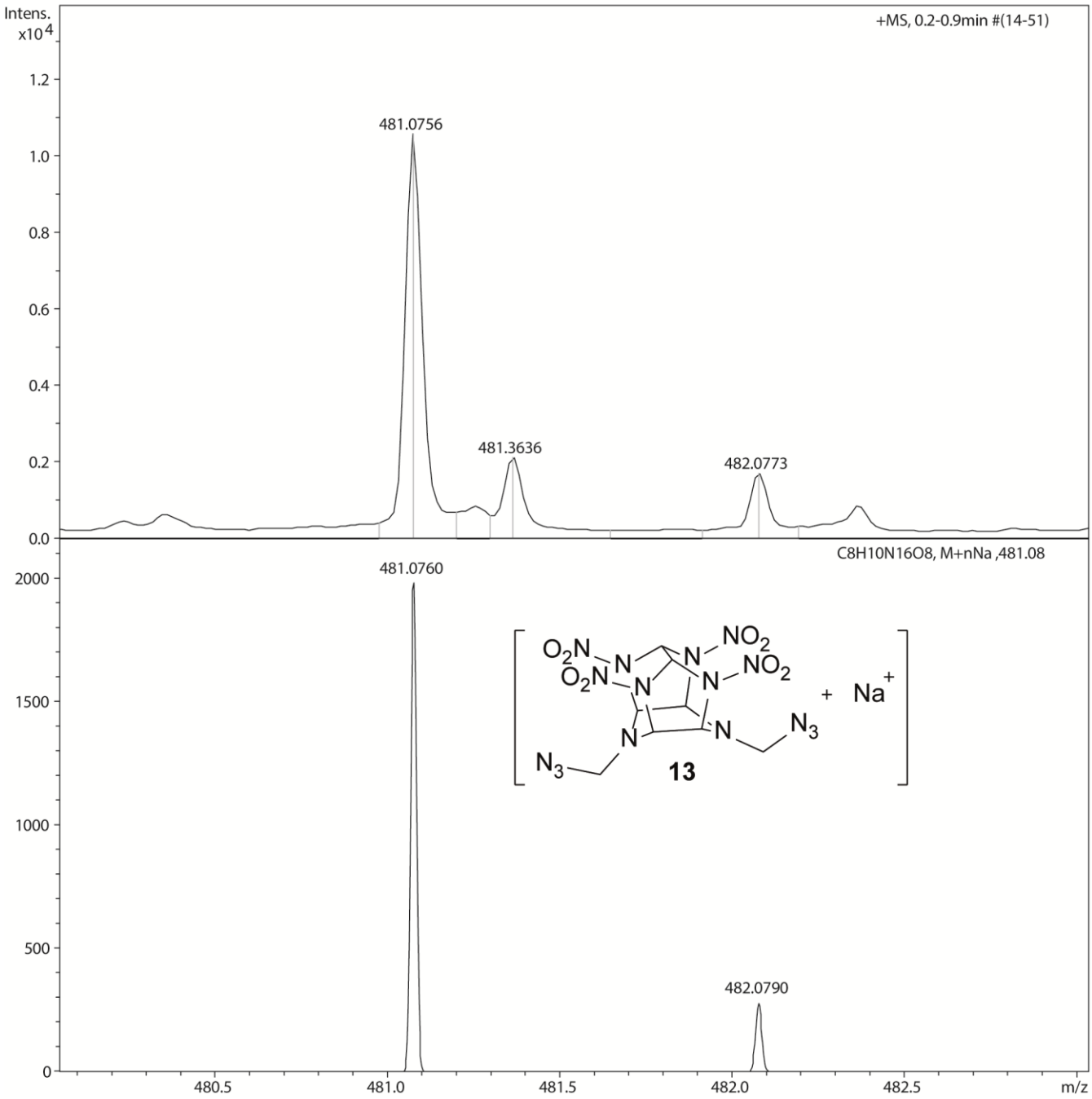
## $^{15}$N NMR ([INVGATED],30.4 MHz,[$D_6$]DMSO) spectrum of compound 13



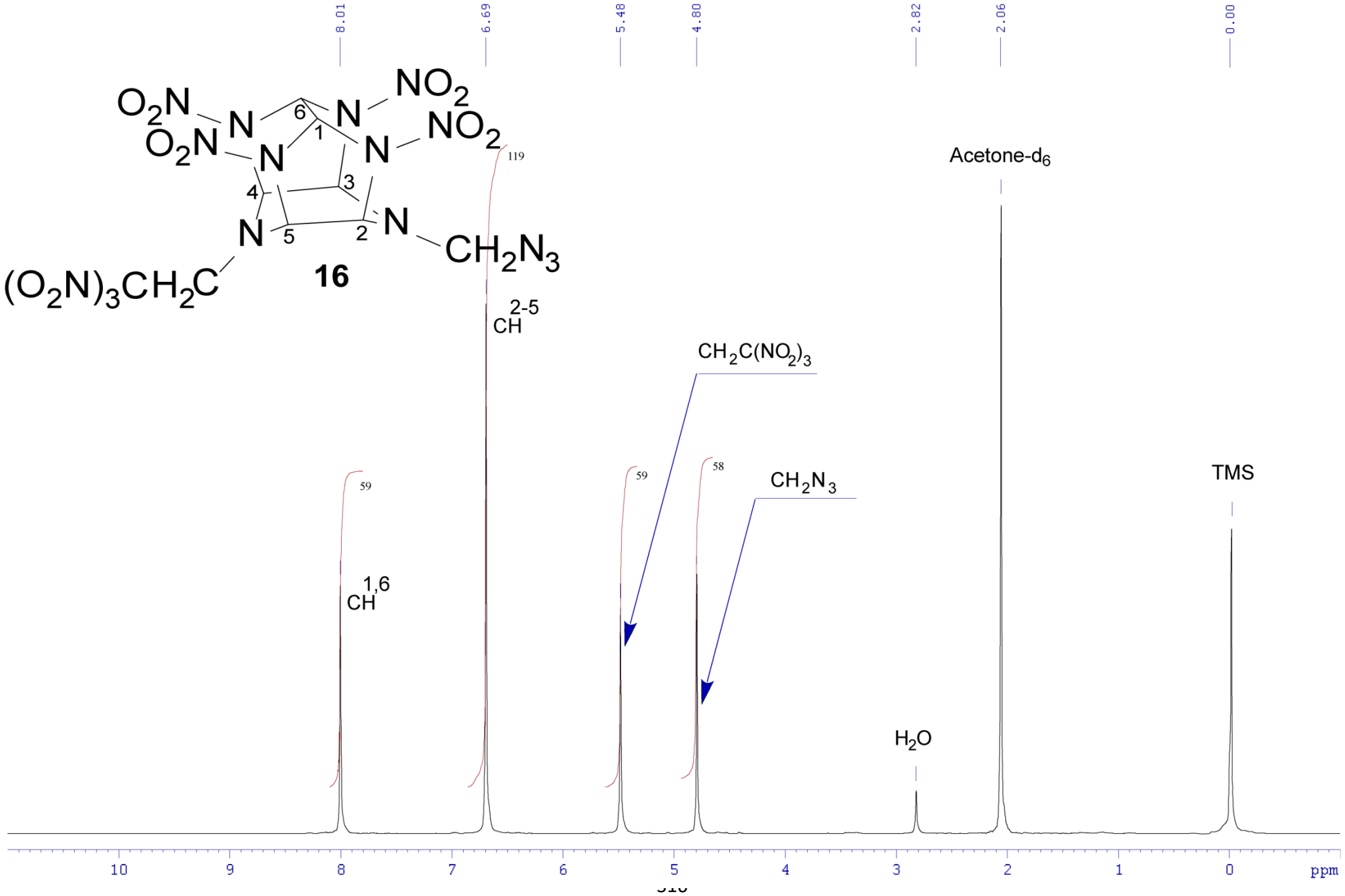
# IR (KBr) spectrum of compound 13



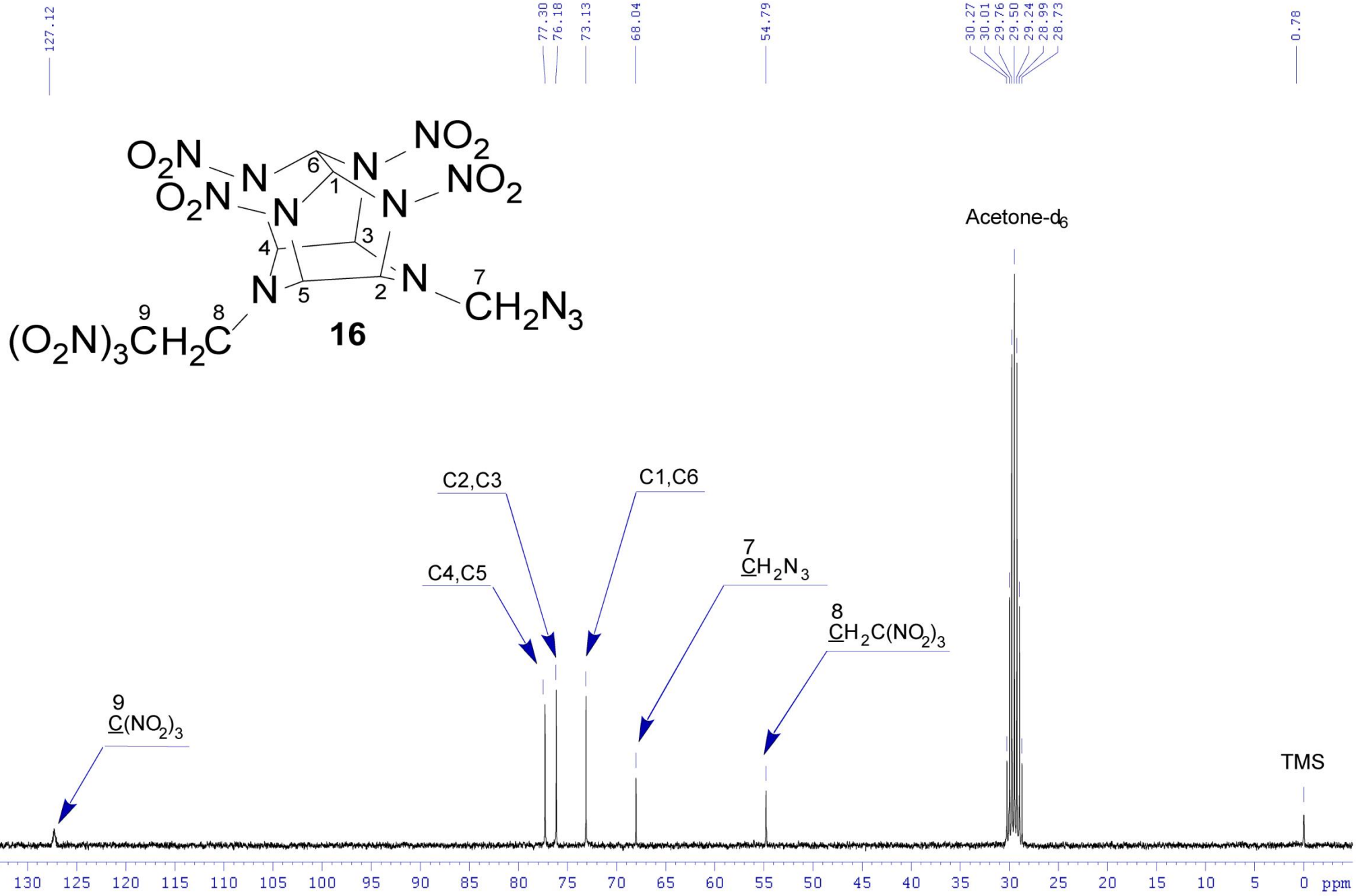
# HRMS (ESI) for compound 13



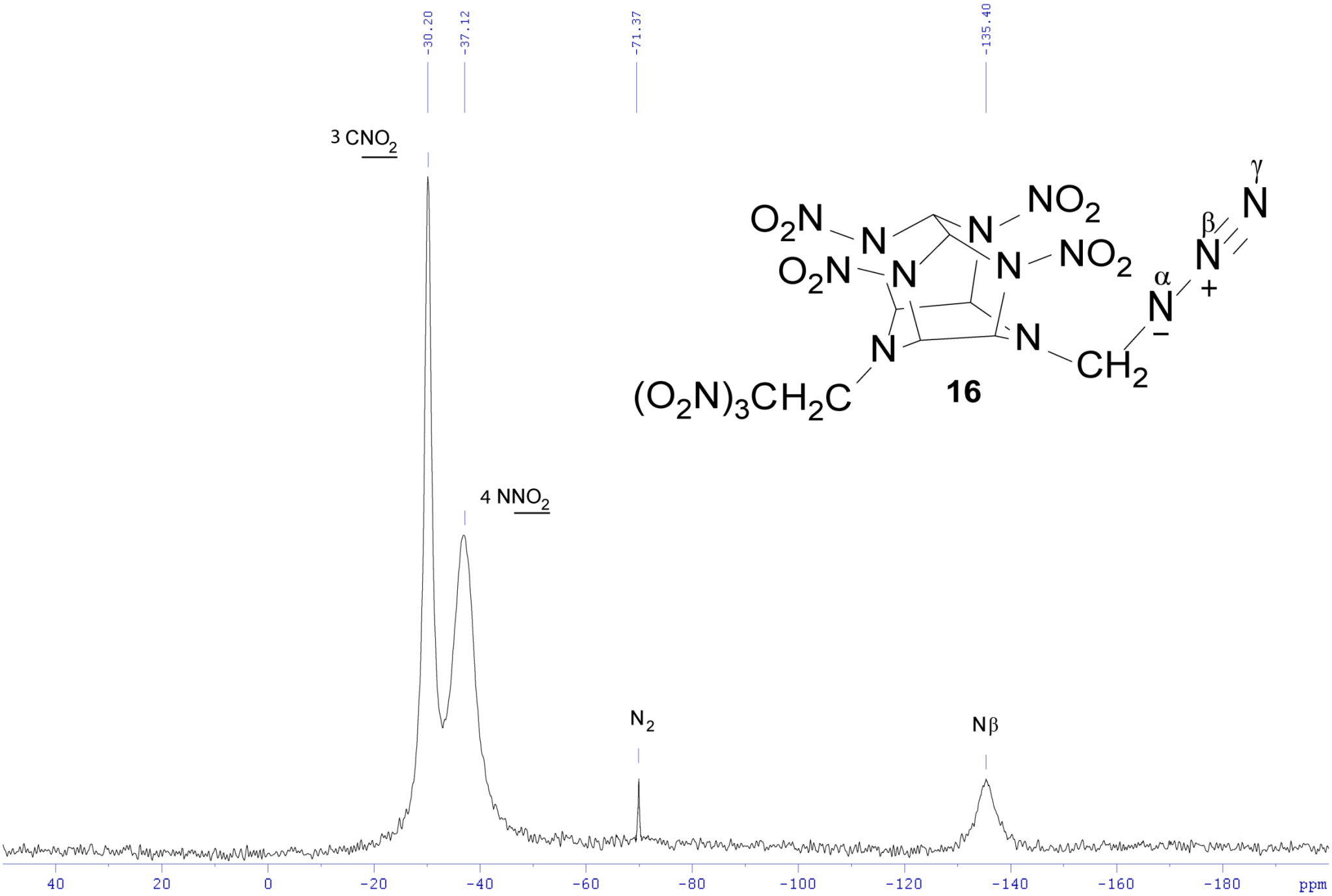
# $^1$H NMR (300.1 MHz, [D$_6$]acetone) spectrum of compound 16



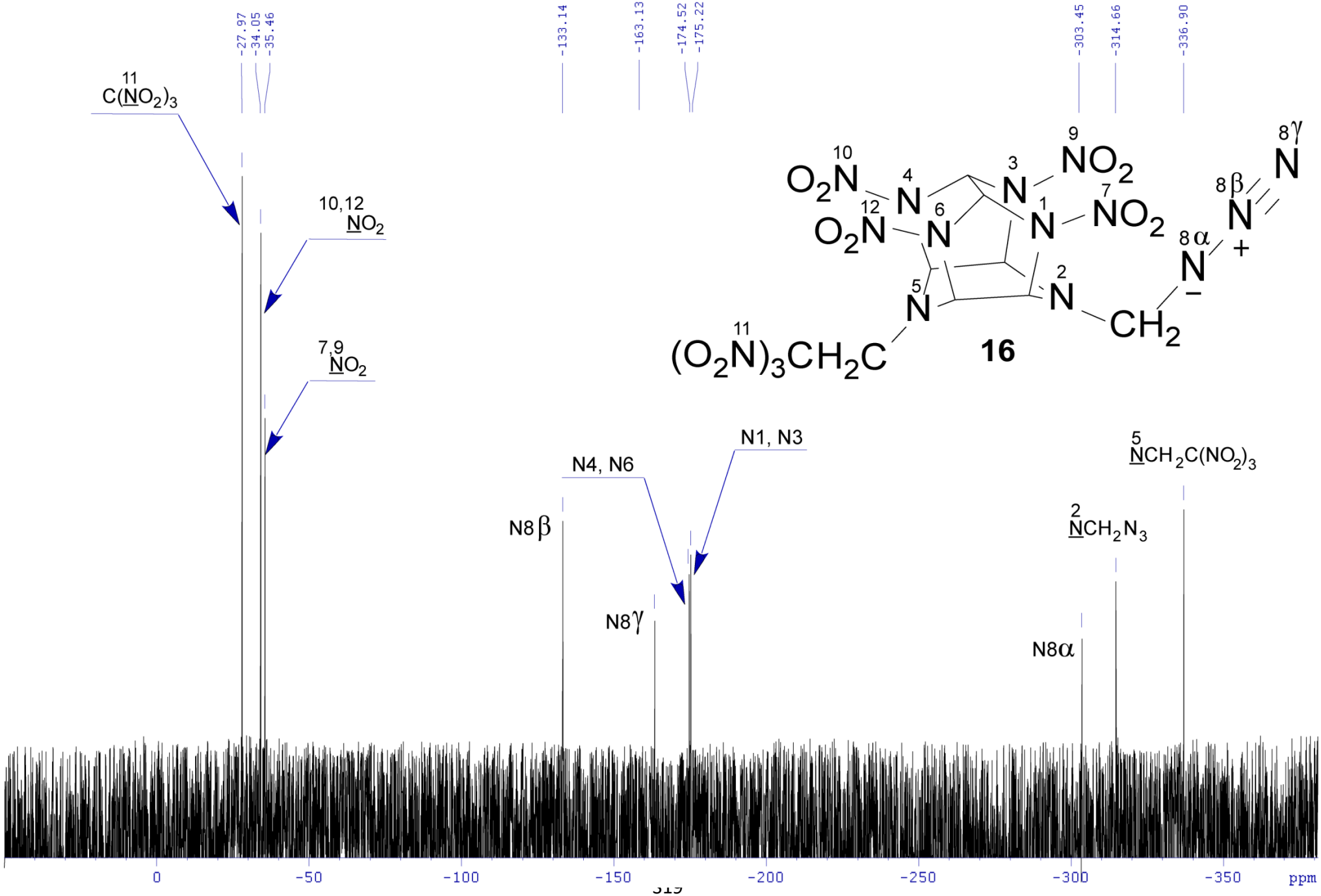
# $^{13}$C NMR (75.5 MHz, [D$_6$]acetone) spectrum of compound 16



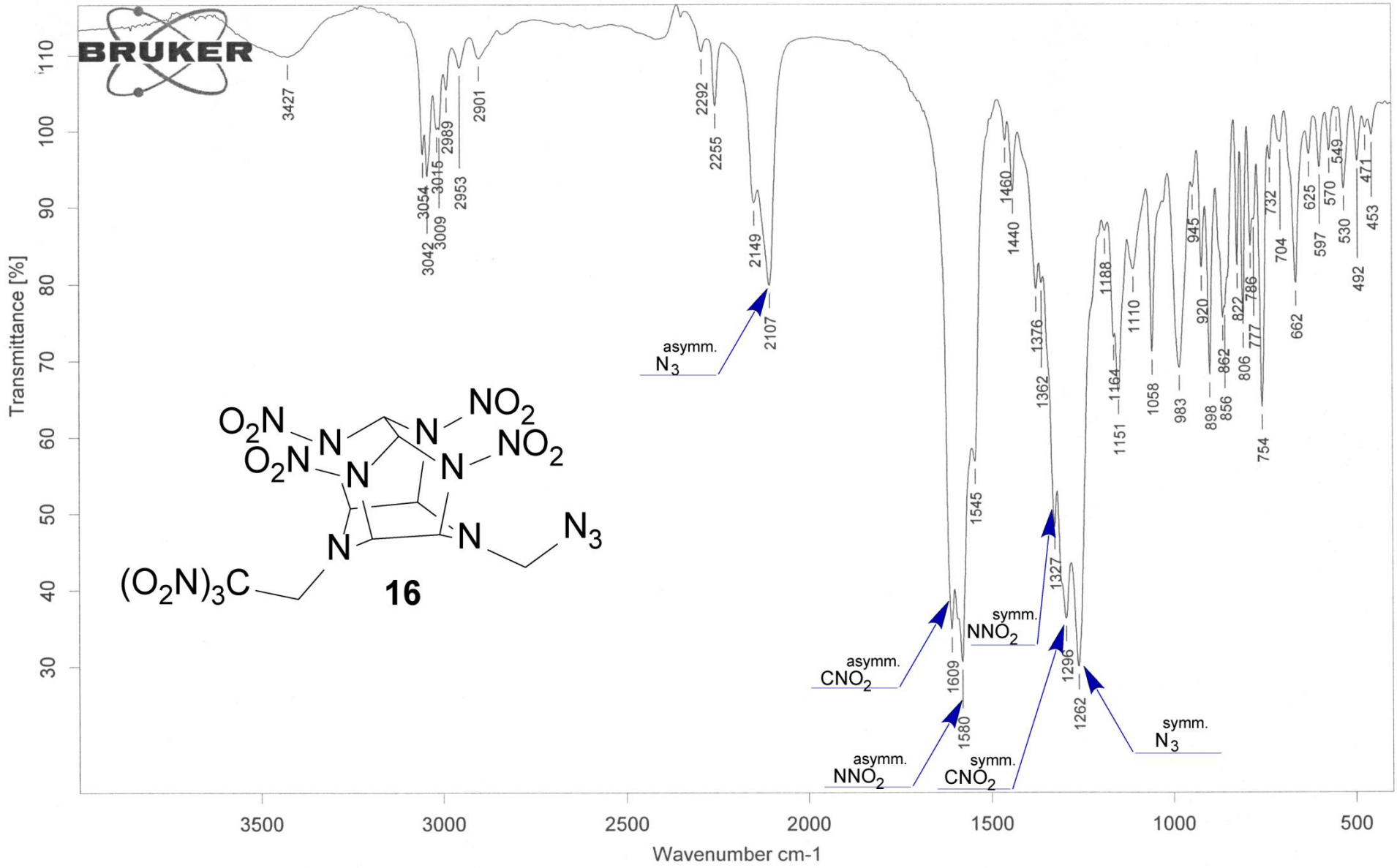
# $^{14}$N NMR (21.7 MHz, [D$_6$]acetone) spectrum of compound 16



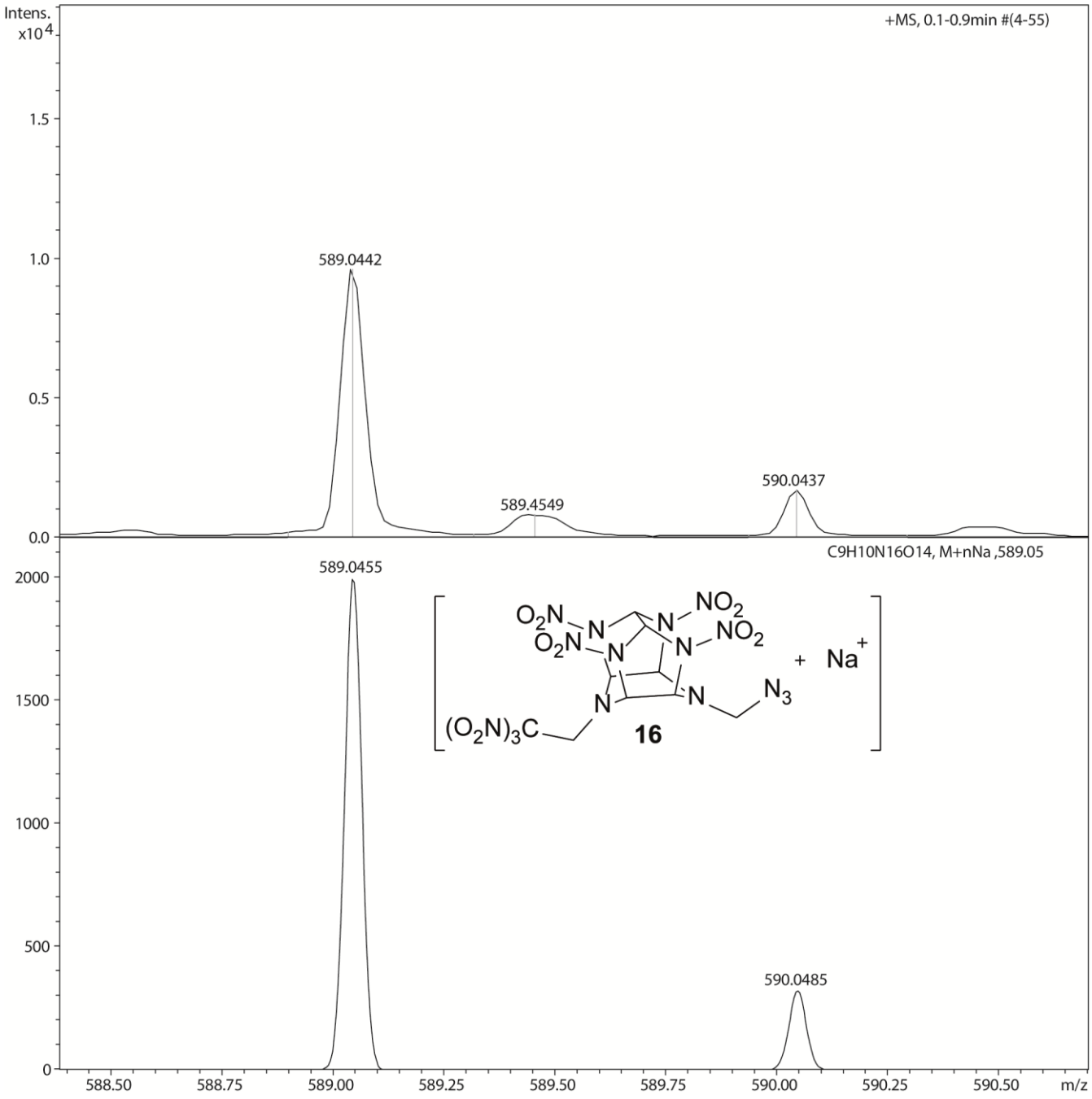
# $^{15}$N NMR ([INVGATED],30.4 MHz,[$D_6$]acetone) spectrum of compound 16



# IR (KBr) spectrum of compound 16



# HRMS (ESI) for compound 16



# X-ray crystal structure determination

## 1) Powder X-ray diffraction of compound 11

The X-ray powder diffraction pattern of compound **9** was measured using CuK*α*1 radiation in transmission mode on a Bruker D8 Advance Vario diffractometer equipped with LynxEye 1D detector and $Ge^{111}$ monochromator. The pattern was indexed using SVD-Index algorithm in monoclinic syngony; systematic absences, cell volume and molecule volume agreed with space group $P2_1/c$ and Z = 8 (Z' = 2).

The initial solutions for the structure were obtained by search in the direct space using Parallel Tempering as implemented in FOX. The resulting structure was used as a starting geometry for the DFT calculations in crystal with fixed and optimized unit cell. Optimization results with fixed unit cell were used as the starting geometries and the sources of bond and angle restrains in the Rietveld refinements.

$R_{wp}/R_{wp}'$ / $R_p/R_p'$ / $R_{Bragg}$ = 1.78/4.65 / 1.33/4.67 / 0.65%, the difference curve was featureless and the molecular geometry (except for the hydrogen atoms) preserved well after the unrestrained refinement.

Two independent molecules in the unit cell shows different conformations: one with axial $CH_2N_3$ group and another with equatorial $CH_2N_3$ group.

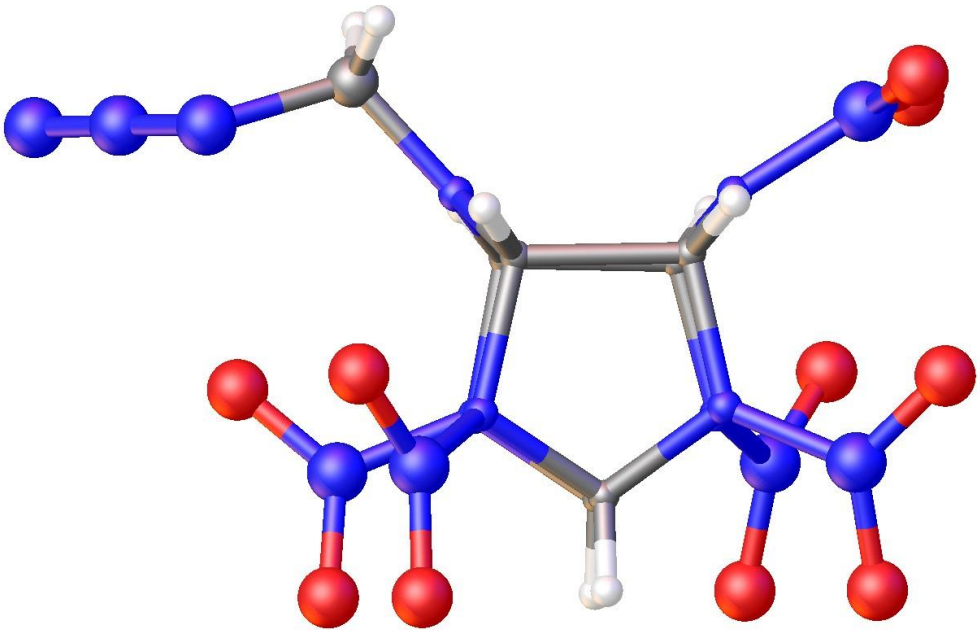


**Figure 1.** View of the first molecule in crystal of compound **11**.

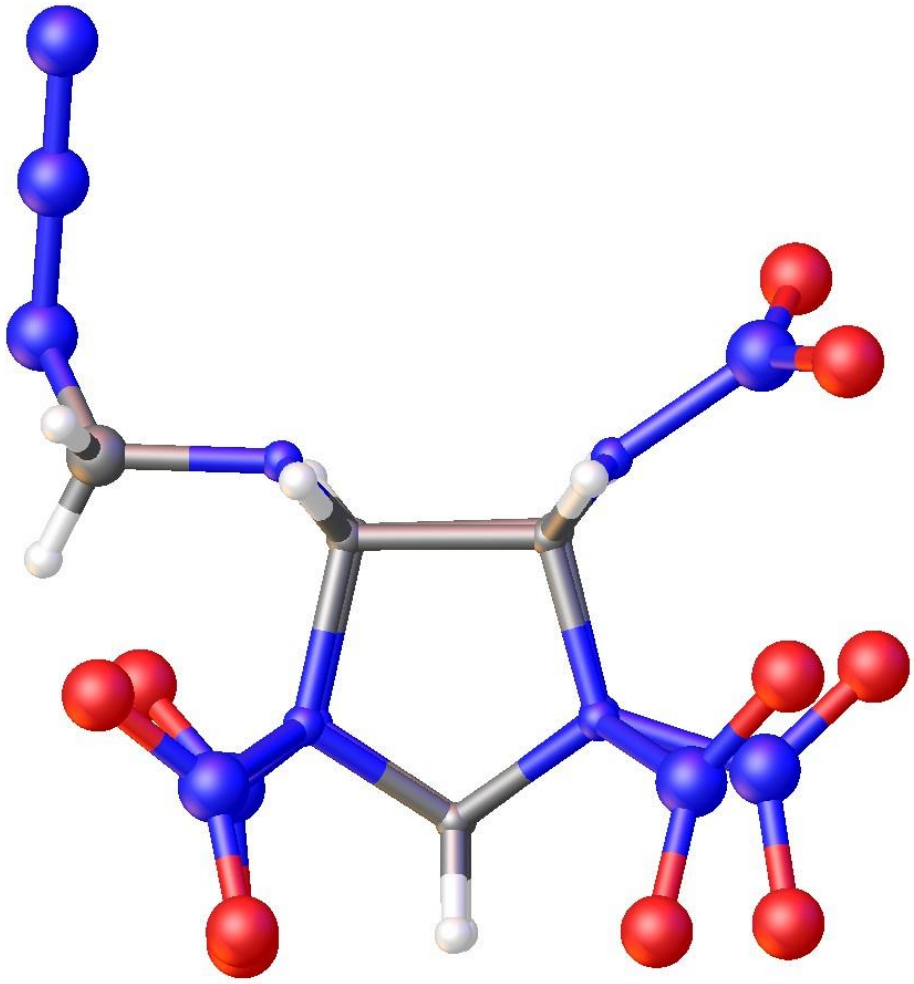


**Figure 2.** View of the second molecule in crystal of compound **11**.

The RMSD of the non-hydrogen atomic positions in the Rietveld refined structure from ones obtained by a calculation with optimized unit cell was 0.08 Å — within the limits proposed by J. van de Streek and M. Neumann for correct powder structures.

Detailed crystallographic information is provided in Table 1. Full crystallographic data have been deposited with the Cambridge Crystallographic Data Center, CCDC 1942572. Copies of the data can be obtained free of charge via https://www.ccdc.cam.ac.uk/structures/.

**Table 1.** Detail Crystallographic data of compounds **11** according to powder X-ray diffraction.

| | |
|---|---|
| Formula | $C_7H_8N_{14}O_1$ |
| Formula weight [g·mol$^{-1}$] | 448.27 |
| Temperature [K] | 298 |
| Radiation | CuKα1 ($\lambda$ = 1.54056) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| Unit cell dimensions | $a$ = 9.8675(3) Å, $\alpha$ = 90°<br>$b$ = 12.6153(3) Å, $\beta$ = 90.7138(6)°<br>$c$ = 24.8333(6) Å, $\gamma$ = 90° |
| $V$ [Å$^3$] | 3091.05(14) |
| $Z$ / $Z'$ | 8 / 2 |
| $\rho_{calc}$ [g·cm$^{-3}$] | 1.927 |
| $\mu$ [mm$^{-1}$] | 1.578 |
| $F$(000) | 1824 |
| $\theta$ range [°] | 2.50 to 45.01 |
| Reflections measured | 8067 |
| Restraints applied/parameters refined | 166 / 227 |
| $R_{wp}$ / $R_{wp}'$ [%] | 1.78 / 4.65 |
| $R_p$ / $R_p'$ [%] | 1.33 / 4.67 |
| $R_{exp}$ [%] | 0.877 |
| $R_I$ [%] | 0.647 |
| CCDC number | 1942572 |

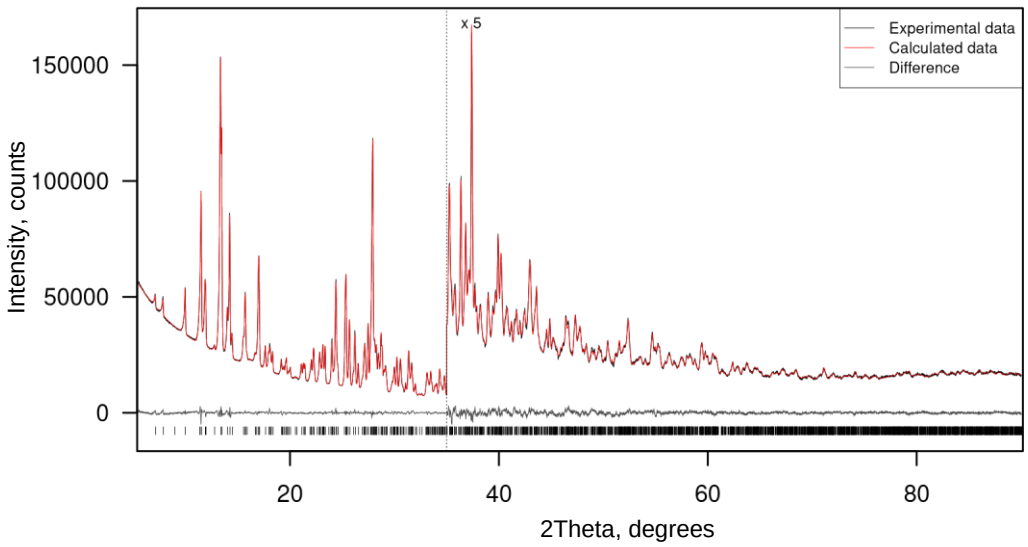



**Figure 3.** Final observed (black), calculated (red) and difference profiles for the Rietveld refinement of compound **11**.

**Table 2.** Selected bond lengths (Å), bond angles (°) and torsion angles (°) of compound **11**.

| **Bond lengths** | |
|---|---|
| *Nitro groups* | |
| N(1)–N(2) / N(1′)–N(2′) | 1.361(19) / 1.35(2) |
| N(10)–N(11) / N(10′)–N(11′) | 1.420(19) / 1.407(18) |
| N(5)–N(6) / N(5′)–N(6′) | 1.446(17) / 1.433(17) |
| N(7)–N(8) / N(7′)–N(8′) | 1.381(18) / 1.371(19) |
| N(3)–N(4) / N(3′)–N(4′) | 1.411(19) / 1.414(19) |
| *Azidomethyl group* | |
| N(9)–C(7) / N(9′)–C(7′) | 1.406(19) / 1.438(19) |
| N(12)–C(7) / N(12′)–C(7′) | 1.451(19) / 1.432(19) |
| N(12)–N(13) / N(12′)–N(13′) | 1.222(19) / 1.256(18) |
| N(13)–N(14) / N(13′)–N(14′) | 1.194(17) / 1.150(18) |
| *Framework* | |
| N(2)–C(1) / N(2′)–C(1′) | 1.458(16) / 1.481(19) |
| N(2)–C(6) / N(2′)–C(6′) | 1.462(19) / 1.462(19) |
| N(10)–C(6) / N(10′)–C(6′) | 1.463(16) / 1.463(17) |
| N(10)–C(5) / N(10′)–C(5′) | 1.491(18) / 1.497(18) |
| C(1)–C(5) / C(1′)–C(5′) | 1.610(19) / 1.573(19) |
| C(3)–C(6) / C(3′)–C(6′) | 1.587(19) / 1.594(19) |
| N(9)–C(4) / N(9′)–C(4′) | 1.442(19) / 1.441(18) |
| N(9)–C(5) / N(9′)–C(5′) | 1.420(18) / 1.444(18) |
| N(3)–C(1) / N(3′)–C(1′) | 1.446(18) / 1.433(18) |
| N(3)–C(2) / N(3′)–C(2′) | 1.421(19) / 1.423(19) |

**Table 2** (continued)

| **Bond angles** | |
|---|---|
| *Nitro groups* | |
| N(1)–N(2)–C(1) / N(1′)–N(2′)–C(1′) | 125.1(13) / 121.3(11) |
| N(1)–N(2)–C(6) / N(1′)–N(2′)–C(6′) | 123.7(11) / 121.4(11) |
| N(11)–N(10)–C(5) / N(11′)–N(10′)–C(5′) | 118.3(10) / 119.1(11) |
| N(11)–N(10)–C(6) / N(11′)–N(10′)–C(6′) | 116.4(10) / 118.1(11) |
| N(6)–N(5)–C(2) / N(6′)–N(5′)–C(2′) | 115.6(11) / 119.0(11) |
| N(6)–N(5)–C(3) / N(6′)–N(5′)–C(3′) | 114.9(11) / 118.1(12) |
| N(8)–N(7)–C(3) / N(8′)–N(7′)–C(3′) | 119.1(11) / 118.7(12) |
| N(8)–N(7)–C(4) / N(8′)–N(7′)–C(4′) | 121.9(11) / 119.9(12) |
| N(4)–N(3)–C(1) / N(4′)–N(3′)–C(1′) | 119.5(13) / 120.4(12) |
| N(4)–N(3)–C(2) / N(4′)–N(3′)–C(2′) | 119.8(11) / 119.5(12) |
| *Azidomethyl group* | |
| C(4)–N(9)–C(7) / C(4′)–N(9′)–C(7′) | 122.2(12) / 112.2(11) |
| C(5)–N(9)–C(7) / C(5′)–N(9′)–C(7′) | 122.3(11) / 111.8(11) |
| N(9)–C(7)–N(12) / N(9′)–C(7′)–N(12′) | 115.6(12) / 109.9(12) |
| N(13)–N(12)–C(7) / N(13′)–N(12′)–C(7′) | 114.9(13) / 113.2(12) |
| N(12)–N(13)–N(14) / N(12′)–N(13′)–N(14′) | 179(3) / 178.9(14) |
| *Framework* | |
| C(1)–N(2)–C(6) / C(1′)–N(2′)–C(6′) | 110.9(11) / 110.4(11) |
| N(2)–C(6)–N(10) / N(2′)–C(6′)–N(10′) | 100.5(10) / 99.9(11) |
| C(5)–N(10)–C(6) / C(5′)–N(10′)–C(6′) | 108.1(10) / 108.3(10) |
| N(10)–C(5)–C(1) / N(10′)–C(5′)–C(1′) | 103.6(9) / 104.2(10) |
| N(2)–C(1)–C(5) / N(2′)–C(1′)–C(5′) | 101.4(11) / 101.6(10) |
| N(2)–C(6)–C(3) / N(2′)–C(6′)–C(3′) | 111.2(10) / 111.3(11) |
| N(10)–C(6)–C(3) / N(10′)–C(6′)–C(3′) | 110.3(10) / 110.4(10) |
| N(5)–C(3)–C(6) / N(5′)–C(3′)–C(6′) | 110.0(11) / 108.1(11) |
| N(7)–C(3)–C(6) / N(7′)–C(3′)–C(6′) | 112.3(10) / 109.6(11) |
| N(2)–C(1)–N(3) / N(2′)–C(1′)–N(3′) | 111.2(11) / 111.2(11) |
| **Torsion angles** | |
| N(1)-N(2)-C(1)-C(5) / N(1′)-N(2′)-C(1′)-C(5′) | –161.7(12) / –176.6(12) |
| N(6)-N(5)-C(2)-C(4) / N(6′)-N(5′)-C(2′)-C(4′) | 107.8(13) / –118.5(13) |
| N(11)-N(10)-C(5)-C(1) / N(11′)-N(10′)-C(5′)-C(1′) | 111.9(12) / –115.7(13) |
| N(8)-N(7)-C(4)-C(2) / N(8′)-N(7′)-C(4′)-C(2′) | 174.2(12) / 116.3(13) |
| C(7)-N(9)-C(4)-C(2) / C(7′)-N(9′)-C(4′)-C(2′) | 129.3(13) / –177.9(11) |
| C(7)-N(9)-C(5)-C(1) / C(7′)-N(9′)-C(5′)-C(1′) | –126.9(13) / 176.5(11) |
| N(4)-N(3)-C(1)-C(5) / N(4′)-N(3′)-C(1′)-C(5′) | 147.7(12) / –145.7(12) |
| N(4)-N(3)-C(2)-C(4) / N(4′)-N(3′)-C(2′)-C(4′) | –145.1(12) / 144.4(12) |
| N(13)-N(12)-C(7)-N(9) / N(13′)-N(12′)-C(7′)-N(9′) | –107.0(15) / –77.9(15) |

**Table 2** (continued)

| | |
|---|---|
| N(2)-C(1)-C(5)-N(10) / N(2′)-C(1′)-C(5′)-N(10′) | –0.7(13) / 1.2(12) |
| C(1)-N(2)-C(6)-C(3) / C(1′)-N(2′)-C(6′)-C(3′) | 77.6(12) / –77.3(13) |
| N(3)-C(1)-C(5)-N(9) / N(3′)-C(1′)-C(5′)-N(9′) | –2.8(14) / 2.4(15) |
| N(3)-C(2)-C(4)-N(9) / N(3′)-C(2′)-C(4′)-N(9′) | –2.5(15) / 0.4(15) |
| C(2)-N(5)-C(3)-C(6) / C(2′)-N(5′)-C(3′)-C(6′) | –79.7(13) / 82.0(12) |
| N(5)-C(2)-C(4)-N(7) / N(5′)-C(2′)-C(4′)-N(7′) | –3.3(13) / 2.6(13) |
| N(5)-C(3)-C(6)-N(2) / N(5′)-C(3′)-C(6′)-N(2′) | 1.4(14) / –2.3(15) |
| C(3)-N(5)-C(2)-C(4) / C(3′)-N(5′)-C(2′)-C(4′) | –22.3(14) / 19.3(14) |
| C(3)-N(7)-C(4)-C(2) / C(3′)-N(7′)-C(4′)-C(2′) | 28.2(13) / –23.8(13) |
| N(7)-C(3)-C(6)-N(2) / N(7′)-C(3′)-C(6′)-N(2′) | –109.2(12) / 110.3(12) |
| N(7)-C(3)-C(6)-N(10) / N(7′)-C(3′)-C(6′)-N(10′) | 1.4(15) / 0.3(16) |
| C(6)-N(2)-C(1)-N(3) / C(6′)-N(2′)-C(1′)-N(3′) | –90.2(14) / 91.3(13) |
| C(6)-N(2)-C(1)-C(5) / C(6′)-N(2′)-C(1′)-C(5′) | 24.8(13) / –25.3(13) |
| C(5)-N(9)-C(7)-N(12) / C(5′)-N(9′)-C(7′)-N(12′) | –75.6(17) / –67.9(14) |
| C(5)-N(10)-C(6)-C(3) / C(5′)-N(10′)-C(6′)-C(3′) | –80.1(12) / 80.0(13) |
| C(4)-N(7)-C(3)-C(6) / C(4′)-N(7′)-C(3′)-C(6′) | 74.3(13) / –78.9(13) |
| C(4)-N(9)-C(7)-N(12) / C(4′)-N(9′)-C(7′)-N(12′) | 101.9(15) / 162.6(11) |

## 2) Single crystal X-ray diffraction of compound 13

X-ray diffraction study of compound **13** was carried out on a «Bruker APEX2 DUO CCD» diffractometer (MoKα radiation: λ = 0.71073 Å, graphite monochromator) at 293 K. The structures were solved by a direct method and refined by least squares in the anisotropic full-matrix approximation in $F^2_{hkl}$. The positions of hydrogen atoms were calculated geometrically and refined in the isotropic approximation by the riding model. All calculations were performed using the SHELXTL PLUS program package. Detailed crystallographic information is provided in Table 2. Full crystallographic data have been deposited with the Cambridge Crystallographic Data Center, CCDC 1938394. Copies of the data can be obtained free of charge via https://www.ccdc.cam.ac.uk/structures/.

**Table 3.** Detail Crystallographic data of compounds **13** according to single crystal X-ray diffraction analysis.

| | |
|---|---|
| Formula | $C_8H_{10}N_{16}O_8$ |
| Formula weight [g·mol$^{-1}$] | 458.27 |
| Temperature [K] | 296 |
| Radiation | MoKα ($\lambda$ = 0.71073) |
| Crystal system | monoclinic |
| Space group | *C*2/c |
| Unit cell dimensions | *a* = 21.810(2) Å, $\alpha$ = 90°<br>*b* = 6.0891(6) Å, $\beta$ = 125.743(2)°<br>*c* = 15.2289(16) Å, $\gamma$ = 90° |
| *V* [Å$^3$] | 1641.5(3) |
| *Z* / *Z*′ | 4 / 1 |
| $\rho_{calc}$ [g·cm$^{-3}$] | 1.854 |
| $\mu$ [mm$^{-1}$] | 0.164 |
| *F*(000) | 937 |
| crystal colour | colourless |
| crystal size [mm$^3$] | 0.35 × 0.30 × 0.35 |
| $\theta$ range [°] | 2.30° to 30.45° |
| Index ranges | –30 ≤ *h* ≤ 25, 0 ≤ *k* ≤ 8, 0 ≤ *l* ≤ 21 |
| Reflections measured | 10816 |
| Independent reflections | 2493 [*R*(int) = 0.0442] |
| Restraints applied/parameters refined | 0 / 165 |
| Goodness-of-fit on $F^2$ | 1.018 |
| Rflections with $I > 2\sigma(I)$ | 1836 |
| Final *R* indeces [$I \geq 2\sigma(I)$] | $R_1$ = 0.0442 , $wR_2$ = 0.1096 |
| Final *R* indeces [all data] | $R_1$ = 0.0637, $wR_2$ = 0.1224 |
| Residual electron density ($\rho_{max}/\rho_{min}$) [e Å$^{-3}$/ e Å$^{-3}$] | 0.341 / –0.264 |
| CCDC number | 1938394 |

**Table 4.** Selected bond lengths (Å) and bond angles (°) of compound **13**

| Bond lengths | |
|---|---|
| *Nitro groups* | |
| N(1)–N(7) | 1.3878(16) |
| N(8)–N(3) | 1.3799(16) |
| | |
| *Azidomethyl groups* | |
| N(2)–C(7) | 1.4507(19) |
| N(4)–C(7) | 1.484(2) |
| N(5)–N(4) | 1.2258(19) |
| N(5)–N(6) | 1.122(2) |
| | |
| N(1)–C(1)` | 1.4492(18) |
| N(3)–C(1) | 1.4551(18) |
| N(3)–C(5) | 1.4907(18) |
| C(3)–C(5) | 1.575(2) |
| N(1)–C(3) | 1.4835(18) |
| C(1)–C(1) | 1.588(3) |
| N(2)–C(5) | 1.4406(18) |
| | |
| Bond angles | |
| *Nitro groups* | |
| C(1)–N(1)–N(7) | 119.55(12) |
| C(3)–N(1)–N(7) | 120.06(11) |
| C(1)–N(3)–N(8) | 118.70(11) |
| C(5)–N(3)–N(8) | 119.24(11) |
| | |
| *Azidomethyl groups* | |
| C(7)–N(2)–C(5) | 115.90(12) |
| N(4)–C(7)–N(2) | 111.61(13) |
| C(7)–N(4)–N(5) | 114.63(15) |
| N(6)–N(5)–N(4) | 173.8(2) |
| | |
| *Framework* | |
| C(3)–N(1)–C(1) | 108.68(11) |
| N(3)–C(1)–N(1) | 103.01(11) |
| C(5)–N(3)–C(1) | 108.23(10) |
| C(3)–C(5)–N(3) | 103.46(11) |
| C(5)–C(3)–N(1) | 103.67(11) |
| | |
| C(1)–C(1)–N(1) | 109.09(12) |
| C(1)–C(1)–N(3) | 108.82(12) |
| C(5)–N(3)–N(8) | 119.24(11) |
| N(3)–C(5)–N(2) | 112.64(11) |
| C(3)–C(5)–N(2) | 110.63(11) |

# Combustion calorimetry measurements of compounds 11 and 13

Measurements were carried out on a precision automatic combustion calorimeter with an isothermal coating specifically developed for combustion of energetic compounds.

The mean square error of the measurements was 0.025%.

**Table 5.** Measurements of combustion energy of compound **11**.

| # | M | $\Delta T$ | $Q$ | $q_a$ | $q_i$ | $q_N$ | $q_{cot}$ | $-\Delta U'_B$ |
|---|---|---|---|---|---|---|---|---|
| **1** | 0.057135 | 2.00210 | 1076.31 | 914.05 | 9.69 | 2.24 | 9.21 | 2469.9 |
| **2** | 0.072369 | 2.07316 | 1114.51 | 918.16 | 5.92 | 2.83 | 9.06 | 2467.1 |
| **3** | 0.078421 | 2.09636 | 1126.98 | 915.60 | 5.88 | 3.04 | 8.47 | 2473.7 |
| **4** | 0.073995 | 2.07470 | 1115.34 | 915.28 | 5.89 | 2.90 | 8.62 | 2468.4 |
| | | | | $-\Delta U'_B$ = 2469.8 ± 3.7 cal·g$^{-1}$ | | | | |
| | | | | **$-\Delta H_c$ = 1099.3 ± 1.7 cal·mol$^{-1}$** | | | | |
| | | | | **$\Delta H_f$ = 167.7 ± 1.7 kcal·mol$^{-1}$** | | | | |

**Table 6.** Measurements of combustion energy of compound **13**.

| # | M | $\Delta T$ | $Q$ | $q_a$ | $q_i$ | $q_N$ | $q_{cot}$ | $-\Delta U'_B$ |
|---|---|---|---|---|---|---|---|---|
| **1** | 0.070302 | 2.11158 | 1135.16 | 912.63 | 5.95 | 2.07 | 8.50 | 2930.4 |
| **2** | 0.072564 | 2.13276 | 1146.55 | 916.88 | 5.92 | 2.21 | 8.66 | 2933.7 |
| **3** | 0.072928 | 2.13484 | 1147.67 | 917.15 | 5.86 | 2.24 | 8.63 | 2931.5 |
| **4** | 0.074012 | 2.13084 | 1145.52 | 911.92 | 5.87 | 2.24 | 8.72 | 2028.8 |
| | | | | $-U'_B$ =2931.0 ± 3.0 cal·g$^{-1}$ | | | | |
| | | | | **$-\Delta H_c$ = 1335.0 ± 1.0 cal·mol$^{-1}$** | | | | |
| | | | | **$\Delta H_f$ = 241.0 ± 1.0 kcal·mol$^{-1}$** | | | | |

The energy equivalent $W = Q_{meas} \cdot \Delta T^{-1}$ was found to be 537.59±0.14 cal·deg$^{-1}$ The combustion energy of the cotton thread measured in a series of seven experiments was 3968.9±1.6 cal·g$^{-1}$.

The standard enthalpies of formation of combustion products are assumed to be as follows:

$\Delta H_f$ $[CO_2]_{(g)}$ = − 94.051 ± 0.031 kcal·mol$^{-1}$,

$\Delta H_f$ $[H_2O]_{(l)}$ = − 68.315 ± 0.009 kcal·mol$^{-1}$.

# Energetic performance of compounds 11 and 13

**Table 7** Physicochemical and energetic properties of **11** and **13** in comparison with HMX and CL-20.

| Compound | Formula | $\alpha^{a}$ | H%[b] | $T_{dec}{}^{c}$ [°C] | $d^{d}$ [g·cm$^{-3}$] | $\Delta H_f{}^{e}$ [kJ·kg$^{-1}$ (kJ·mol$^{-1}$)] | $Q_{comb}{}^{e}$ [kJ·kg$^{-1}$] | $D_V{}^{f}$ [km·s$^{-1}$][e] | $P_{C\text{-}J}{}^{f}$ [GPa][e] |
|---|---|---|---|---|---|---|---|---|---|
| **11** | $C_7H_8N_{14}O_{10}$ | 0.56 | 1.79 | 206 | 1.927 | +1568 (+702) | 10281 | 9.12 | 40.5 |
| **13** | $C_8H_{10}N_{16}O_8$ | 0.38 | 2.18 | 179 | 1.854 | +2205 (+1010) | 12213 | 9.17 | 39.2 |
| β-HMX[g] | $C_4H_8N_8O_8$ | 0.67 | 2.70 | 280 | 1.905 | +255 (+76) | 9448 | 9.23 | 40.7 |
| ε-CL-20[g] | $C_6H_6N_{12}O_{12}$ | 0.80 | 1.37 | 229 | 2.044 | +857 (+375) | 8215 | 9.49 | 47.0 |

[a] Oxygen coefficient. For a compound with the molecular formula C*x*H*y*N*w*O*z*, $\alpha = z/(2x+y/2)$. [b] Hydrogen content. [c] Decomposition onset temperature at a heating rate of 5 °C·min$^{-1}$ (DSC). [d] Density measured by X-ray diffraction at 25 °C. [e] Enthalpy of formation and heat of combustion in oxygen determined by the method of combustion calorimetry. [f] Detonation parameters: velocity and pressure calculated with *S&DV4.5* code. [g] R. Meyer, J. Kohler and A. Homburg, *Explosives*, 7th edition, Wiley-VCH, Weinheim, 2016.