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Polynitropyrazole derivatives of pentanitroisowurtzitane

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Contents

Experimental Section

IR spectra were recorded on FTIR spectrometer InfraLUM FT-08 by Lumex in the range from 4000 to 400 cm–1 (resolution 2 cm^{-1}) by using NPVO method. NMR were recorded on ^{1}H, ^{13}C and ^{14}N NMR spectra were recorded at 299 K using a 300 MHz (Bruker AM300) nuclear magnetic resonance spectrometer operating at 300.1, 75.5 and 30.4, respectively, or ^{1}H, $^{13}C\{^{1}H\}$, ^{14}N and ^{15}N NMR spectra were recorded using a 600 MHz (Bruker AV600) nuclear magnetic resonance spectrometer operating at 600.13, 564,69, 150.9, 43.37 and 60.8 MHz, respectively. Acetone-d_6 was employed as NMR solvent (unless specifically agreed). Chemical shifts in the ^{1}H, ^{13}C, ^{14}N and ^{15}N spectra are reported in delta (δ) units, parts per million (ppm), relative to the internal standard Me_4Si (TMS) (^{1}H, ^{13}C – positive values correspond to downfield chemical shifts) and external standard $MeNO_2$ (^{14}N, ^{15}N – negative values correspond to upfield shifts). The values of the spectral parameters J are given in Hz. High-resolution mass spectra (HRMS) were recorded by electrospray ionization (ESI) with a Bruker micrOTOF II instrument. Elemental analyses were carried out on Perkin Elmer 2400 elemental analyzer. Thermochemical measurements compounds **4a-f** were carried out on a precision automatic combustion calorimeter with an isothermal coating specifically developed for combustion of energetic compounds. Thermal behavior was studied with simultaneous thermal analysis STA 449 F1 Jupiter (Netzsch). A sample with a mass of 0.1-0.5 mg was placed into capped aluminum crucibles with cracked lids and heated at a linear rate of 5 $K \cdot min^{-1}$ in argon flow under atmospheric pressure. Sensitivity toward impact and friction was measured on a BAM devices using STANAG standards. The powders densities compounds **4a-e** were measured at 302 K using a Micromeritics AccuPyc II 1340 V3.0 helium pycnometer. Analytical thin-layer chromatography (TLC) was carried out on Silufol UV-254 silica gel aluminum foil. The compounds **4a-f** were purified using preparative thin-layer chromatography on silica gel Merck 60 (15–40 μm), used as eluent mix. EtAc/Hex in a ratio of 1 to 2 or 2 to 3. Melting points were determined with a Boethius Kofler melting point apparatu s (heat rate 5 $°C \cdot min^{-1}$).

Synthesis of 10-(polynitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitanes 4a-f: Thionyl chloride (8 ml) was added to a mixture of compound **1** (0.25 g, 0.64 mmol) and paraformaldehyde (0.113 g, 3.7 mmol) with stirring and room temperature. The mixture was stirred in a stoppered flask for 24 hours. After that, $SOCl_2$ was removed in vacuum at a temperature of about 30 ° C. The solid residue was dried in vacuum for 30 minutes. After that, the white solid residue was dissolved in abs. acetonitrile and dripped with stirring and room temperature to the pre-prepared mixture 0.64 mmol of the corresponding pyrazole **3a-f** and the corresponding base (0.67 mmol).

The reaction mixture was kept under stirring and at room temperature. The mixture was then evaporated in a vacuum and the remainder was suspended in ethyl acetate (25 ml). The organic suspension was washed with 25 ml of water and dried with $MgSO_4$. The desiccant was removed, the organic extract was evaporated in vacuum, and pyrazole derivatives **4a-f** were isolated from the residue by preparative chromatography (eluent ethyl acetate hexane, 1:2).

Table S1. The influence of the nature of the base on the yield of the compound **4a-e**.

Base	Yield, %				
	4a	**4b**	**4c**	**4d**	**4e**
KOH	60	32	47	39	44
Et_3N	30	45	42	40	56
K_2CO_3	69	65	52	49	87
Na_2CO_3	50	57	57	40	77

10-(4-Nitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane (4a): Colorless needles. Reaction time 24 h. Yield: 30÷69 %. Dec. p. 214 °C. IR : ν = 3036 (m), 1588 (s), 1537 (m), 1510 (m), 1257 (s), 1107 (m), 1071 (m), 1000 (vs), 958 (m), 891 (m), 880 (m), 817 (m), 749 (s), 653 (m), 613 (w), 593 (m), 534 (m), 450 (m) cm^{-1}. ^1H NMR (600.1 MHz, [D6]acetone): δ = 8.85 (s, 1 H, H-5 Pz); 8.19 (s, 1 H, H-3 Pz); 8.06 (s, 2H, 2CH), 7.92 (d, J= 3.5 Hz, 2 H, 2CH), 7.1 (d, J= 3.5 Hz, 2 H, 2CH), 5.84 (s, 2H, CH_2) ppm. ^{13}C NMR (150.9 MHz, [D6]acetone): δ = 147.8 (C(3) Pz); 135.2 (C(5)H Pz); 127.0 (C(4) Pz); 81.6 (CH_2); 41.6 $N(CH_3)_2$) ppm. ^{14}N NMR (43.4 MHz, [D6]acetone): –19.45; –40.40 ppm. ^{15}N NMR ([INVGATED], 60.8 MHz, [D6]acetone):–19.09; –37.95, –40.12, –41.17, –73.09, –162.65, –178.35, –180.94, –199.49, –318.76 ppm. HRMS (ESI): *m/z* calcd for $C_{10}H_{10}N_{14}O_{13}$: 536.0941 $[M+NH_4]^+$, 541.0495 $[M+Na]^+$. *m/z* found: 536.0922 $[M+NH_4]^+$, 541.0478 $[M+Na]^+$.

10-(3,4-Dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane (4b): Almost colorless needles**.** Reaction time 3.5 h. Yield: 32÷65 % Dec. p. 172 °C. IR : ν = 3036 (m), 1583 (s), 1553 (s), 1520 (s), 1236 (m), 1258 (vs), 1175 (w), 1135 (w), 1118 (w), 1074 (w), 1043 (w), 1018 (w), 957 (m), 887 (m), 855 (m), 824 (m), 807 (m), 746 (s), 654 (m), 620 (w), 610 (w), 596 (w), 544 (m), 459 (m) cm^{-1}. ^1H NMR (600.1 MHz, [D6]DMSO): δ = 9.19 (s, 1 H, H-5 Pz); 7.94 (s, 2H, 2CH), 7.66 (d, J= 3.5 Hz, 2 H, 2CH), 6.78 (d, J= 3.5 Hz, 2 H, 2CH), 5.70 (s, 2H, CH_2) ppm. ^{13}C NMR (150.9 MHz, [D6]DMSO): δ =

147.24 (C(3) Pz); 134.21 (C(5)H Pz); 126.35 (C(4) Pz); 75.92 (CH_2); 73.14; 70.07; 68.84 (CH) ppm. ^{14}N NMR (43.4 MHz, [D6]DMSO): δ = –38.97 ppm. ^{15}N NMR ([INVGATED], 60.8 MHz, [D6]DMSO): δ = –26.27; –38.01, –39.91, –40.66, –82.17, –169.61, –178.42, –181.30, –199.13, –320.69 ppm. HRMS (ESI): *m/z* calcd for $C_{10}H_9N_{15}O_{14}$: 581.0792 $[M+NH_4]^+$, 586.0346 $[M+Na]^+$; *m/z* found: 581.0767 $[M+NH_4]^+$, 586.0329 $[M+Na]^+$.

10-(3,5-Dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane (4c): Almost colorless needles**.** Reaction time 3.5 h. Yield: 47÷57 % Dec. p. 204 ºC. IR : ν = 3038 (m), 1572 (vs), 1542 (m), 1514 (s), 1453 (m), 1327 (s), 1262 (vs), 1176 (m), 1136 (m), 1106 (w), 1076 (w), 1036 (w), 999 (w), 960 (w), 929 (w), 910 (w), 884 (s), 855 (s), 826 (m), 806 (m), 757 (s), 741 (s), 680 (m), 662 (m), 602 (w), 584 (w), 530 (m), 484 (w), 457 (w) cm^{-1}. ^{1}H NMR (600.1 MHz, [D6]acetone): δ = 8.09 (s, 2 H, 2 CH); 7.99 (s, H, H-4 Pz), 7.98 (d, J= 3.5 Hz, 2 H, 2CH), 7.16 (d, J= 3.5 Hz, 2 H, 2CH), 6.34 (s, 2H, CH_2) ppm. ^{13}C NMR (150.9 MHz, [D6]acetone): δ = 152.47 (C(3) Pz); 145.40 (C(5)H Pz); 102.72 (C(4) Pz); 76.01 (CH_2); 73.09; 70.31; 68.95 (CH) ppm. ^{14}N NMR (43.4 MHz, [D6]acetone): δ = –31.04, –40.30 ppm. ^{15}N NMR ([INVGATED], 60.8 MHz, [D6]acetone): δ = –25.44; –30.44; –38.30, –38.34, –40.03, –41.21, –72.05 (N(2)–Pz), –170.06, –178.48, –180.31, –198.89 (N(1)–Pz), –320.18 ppm. HRMS (ESI): *m/z* calcd for $C_{10}H_9N_{15}O_{14}$: 581.0792 $[M+NH_4]^+$. $]^+$; *m/z* found:581.0803 $[M+NH_4]^+$.

10-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane (4d): Slightly yellow needles**.** Reaction time 0.25 h. Yield: 39÷49% . Dec. p 162 ºC. IR : ν =: 3457 (m), 3352 (m), 3041 (m), 1623 (m), 1569 (m), 1520 (m), 1472 (m), 1381 (m), 1330 (s), 1251 (vs), 1185 (w), 1160 (w), 1128 (w), 1099 (w), 1077 (w), 1053 (w), 942 (s), 883 (s), 854 (w), 824 (m), 793 (m), 748 (s), 693 (w), 658 (m), 612 (w), 553 (w), 530 (w), 496 (w), 467 (w), 432 (w) cm^{-1}. ^{1}H NMR (600.1 MHz, [D6]acetone): δ = 8.12 (s, 2 H, 2 CH); 7.94 (d, J= 3.5 Hz, 2 H, 2CH), 7.79 (s, 2H, NH_2), 7.10 (d, J= 3.5 Hz, 2 H, 2CH), 5.67 (s, 2H, CH_2) ppm. ^{13}C NMR (150.9 MHz, [D6]acetone): δ = 147.24 (C(3) Pz); 134.21 (C(5)H Pz); 126.35 (C(4) Pz); 75.92 (CH_2); 73.14; 70.07; 68.84 (CH) ppm. ^{14}N NMR (43.4 MHz, [D6]acetone): δ = –24.70; –40.65 ppm. ^{15}N NMR ([INVGATED], 60.8 MHz, [D6]acetone): δ = –23.50; –23.78 –37.64, –37.69, –40.09, –41.28 –105.38 (N(2)–Pz), –178.67, –180.57, –180.75, –200.11 (N(1)–Pz), –208.86 (NH_2) –315.50, –320.62 ppm. HRMS (ESI): *m/z* calcd for $C_{10}H_{10}N_{16}O_{14}$: 596.0901 $[M+NH_4]^+$, 617.0194 $[M+K]^+$; *m/z* found: 596.0890 $[M+NH_4]^+$, 617.0194 $[M+K]^+$.

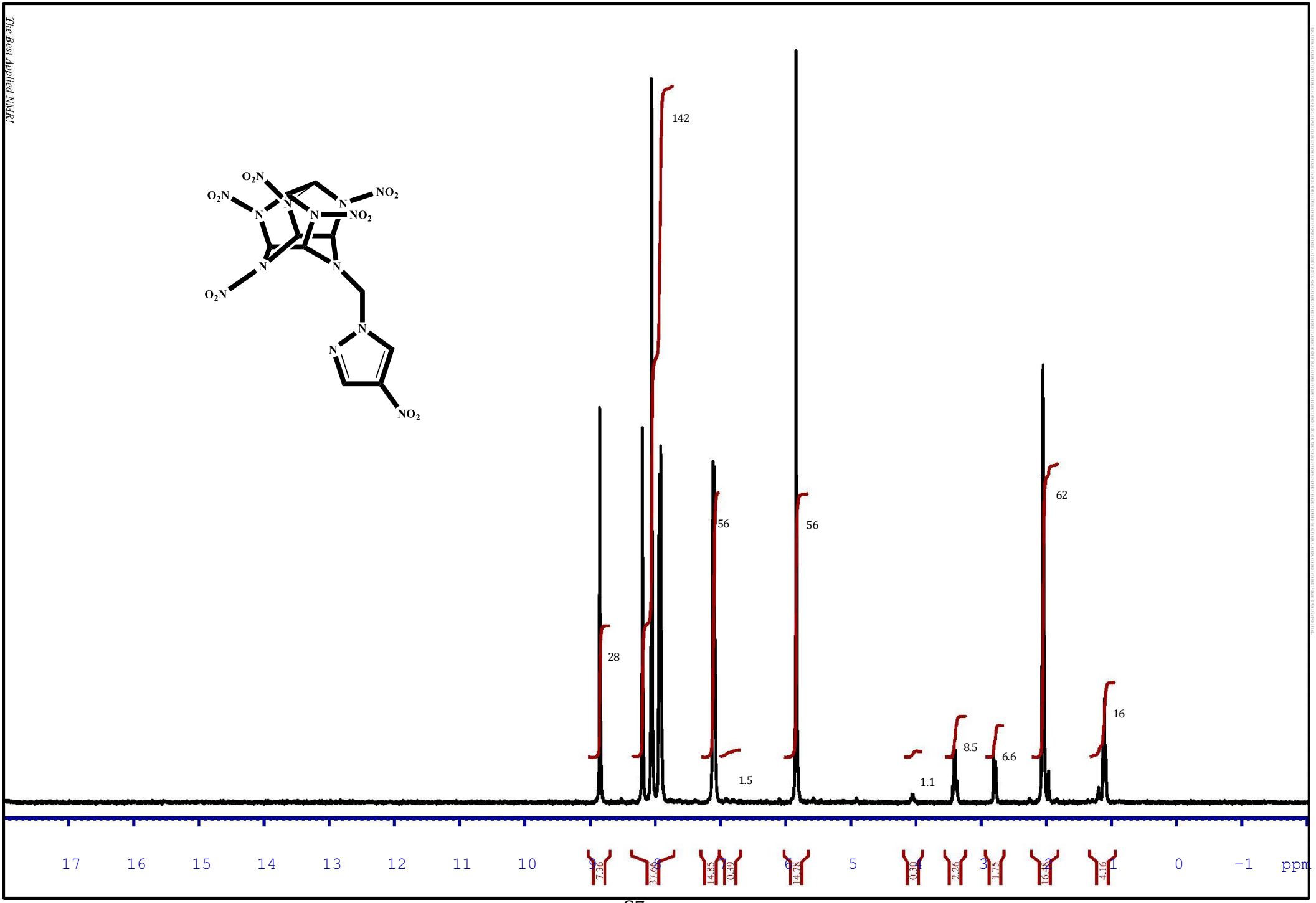
10-(4-Amino-3,5-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane (4e): Lemon yellow needles**.** Reaction time 0.25 h. Yield: 44÷87%.

Dec. p. 209 ºC. IR : ν =: 3506 (m), 3389 (m), 3040 (m), 1649 (w), 1615 (s), 1572 (s), 1508 (m), 1475 (s), 1451 (m), 1415 (w), 1379 (w), 1279 (vs), 1255 (vs), 1172 (m), 1148 (m), 1070 (s), 997 (w), 956 (s), 925 (w), 884 (m), 851 (w), 825 (m), 788 (m), 735 (w), 690 (m), 658 (m), 624 (m), 544 (w), 516 (w) cm^{-1}. . ^{1}H NMR (600.1 MHz, [D6]acetone): δ = 8.05 (s, 2H, 2CH), 7.92 (d, J= 3.5 Hz, 2 H, 2CH), 7.07 (d, J= 3.5 Hz, 2 H, 2CH), 7.06 (br. s, 2H, NH_2), 6.19 (s, 2H, CH_2) ppm. ^{13}C NMR (150.9 MHz, [D6]acetone): δ = 140.96 (C(3) Pz); 130.76 (C(5)H Pz); 130.53 (C(4) Pz); 75.65 (CH_2); 73.14; 70.33; 69.43 (CH) ppm. ^{14}N NMR (43.4 MHz, [D6]acetone): δ = –28.58; –40.54 ppm. ^{15}N NMR ([INVGATED], 60.8 MHz, [D6]acetone): δ = –22.88; –28.29 –38.05, –40.04, –41.01, –72.58 (N(2)–Pz), –178.35, –180.23, –181.51 (NH_2), –198.77 (N(1)–Pz), –318.75, –319.21 ppm. HRMS (ESI): *m/z* calcd for $C_{10}H_{10}N_{16}O_{14}$: 596.0901 $[M+NH_4]^+$, 601.0455 $[M+Na]^+$; *m/z* found: 596.0910 $[M+NH_4]^+$, 601.0458 $[M+Na]^+$.

10-(5-Chloro-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane (4f): Almost colorless needles**.** Reaction time 3.5 h. Выход 20%. Dec. p. 211 ºC. IR : ν = 3037 (m), 1705 (m), 1586 (s), 1541 (s), 1509 (s), 1471 (w), 1429 (w), 1359 (m), 1326 (s), 1255 (vs), 1169 (m), 1138 (w), 1053 (m), 955 (s), 881 (s), 853 (w), 812 (m), 790 (s), 654 (w), 619 (w), 562 (w), 529 (w), 455 (m) cm^{-1}. ^{1}H NMR (300.1 MHz, [D6]acetone): δ = 8.10 (s, 2H, 2CH), 8.04 (d, J= 4 Hz, 2 H, 2CH), 7.17 (d, J= 4 Hz, 2 H, 2CH), 6.09 (s, 2H, CH_2) ppm. ^{13}C NMR (150.9 MHz, [D6]acetone): δ = 147.50 (C(3) Pz); 130.00 (C(5)H Pz); 123.70 (C(4) Pz); 80.06 (CH_2); 75.77; 73.27; 70.20; 64.82 (CH) ppm. ^{14}N NMR (43.4 MHz, [D6]acetone): δ = –27.96; –40.08 ppm. HRMS (ESI): *m/z* calcd for $C_{10}H_8N_{15}O_{14}Cl$: 619.9956, 621.9928 $[M+Na]^+$, 635.9695, 637.9658 $[M+K]^+$; *m/z* found: 619.9979, 621.9957 $[M+Na]^+$, 635.9718, 637.9761 $[M+K]^+$.

Spectral data of compounds 4a-f.

^{1}H-NMR, ^{13}C-NMR, ^{14}N-NMR, ^{15}N-NMR.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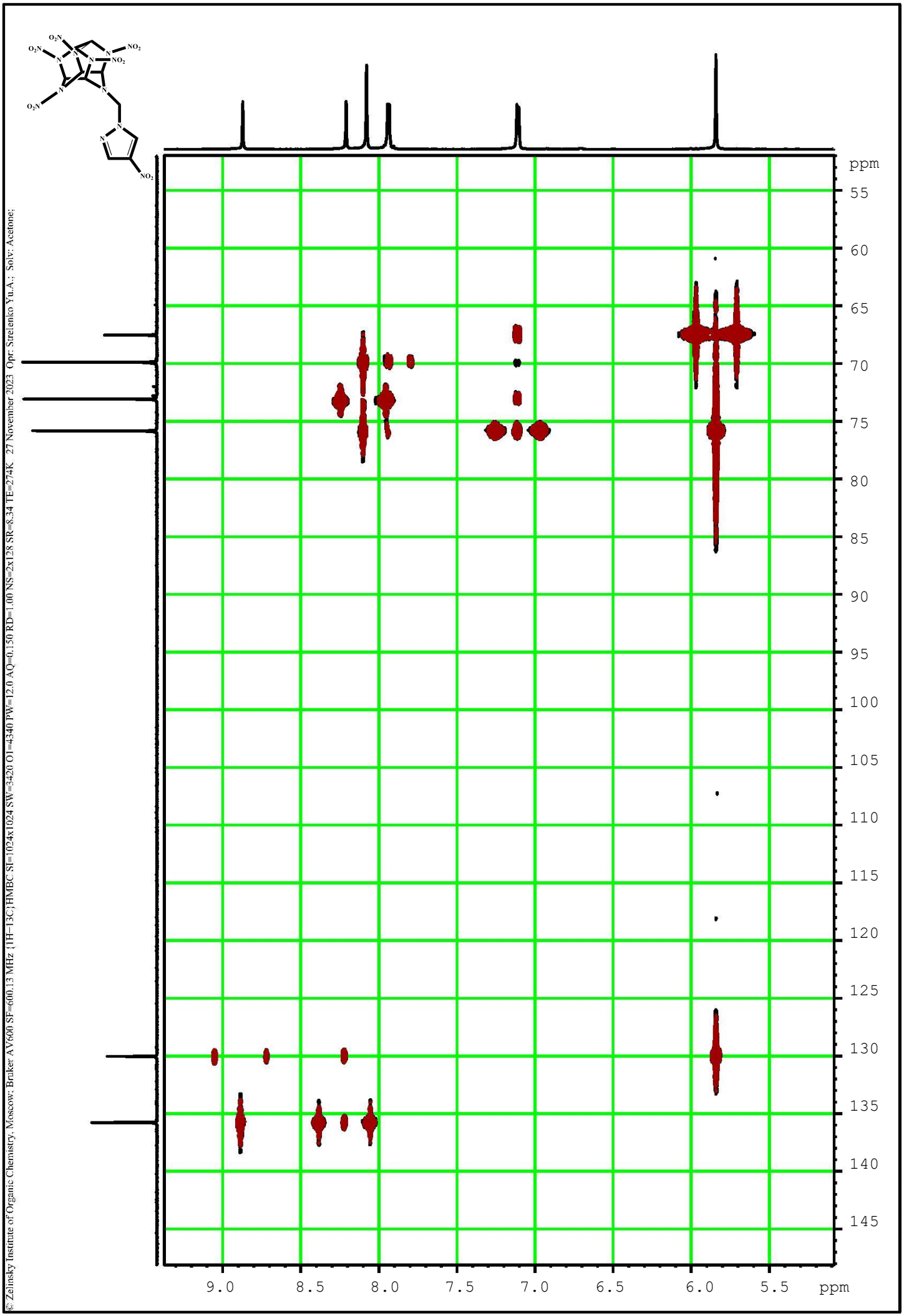
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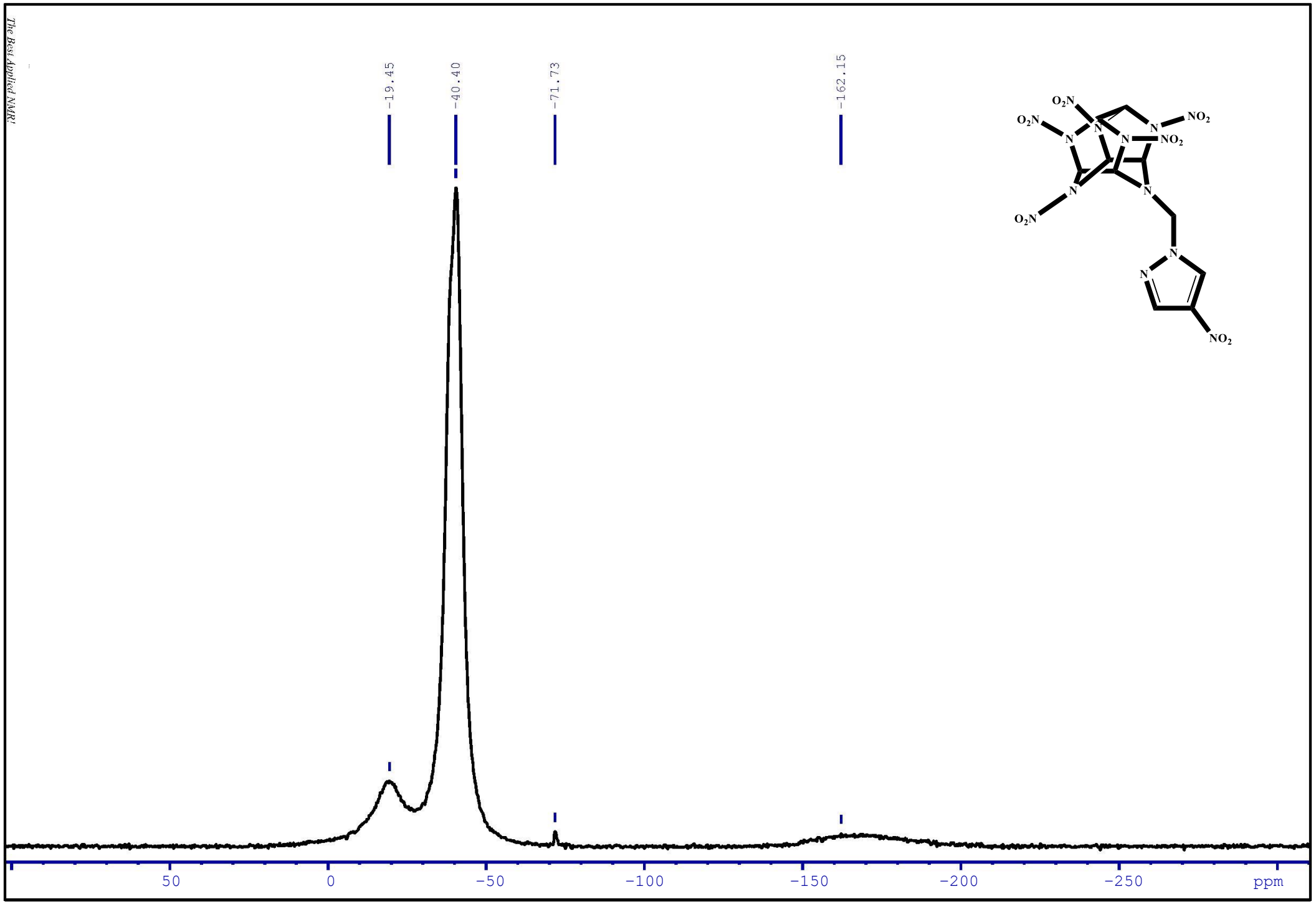
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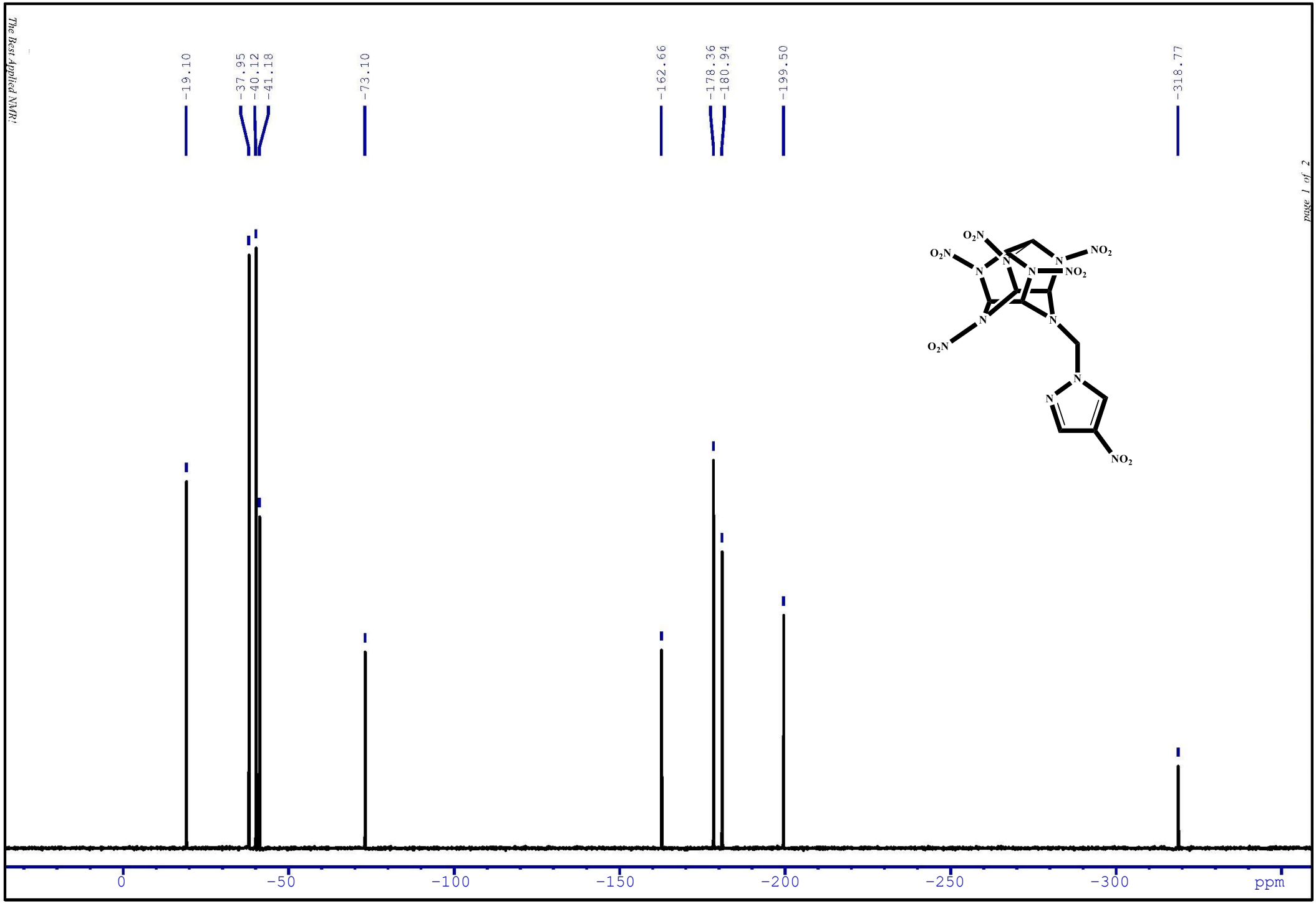
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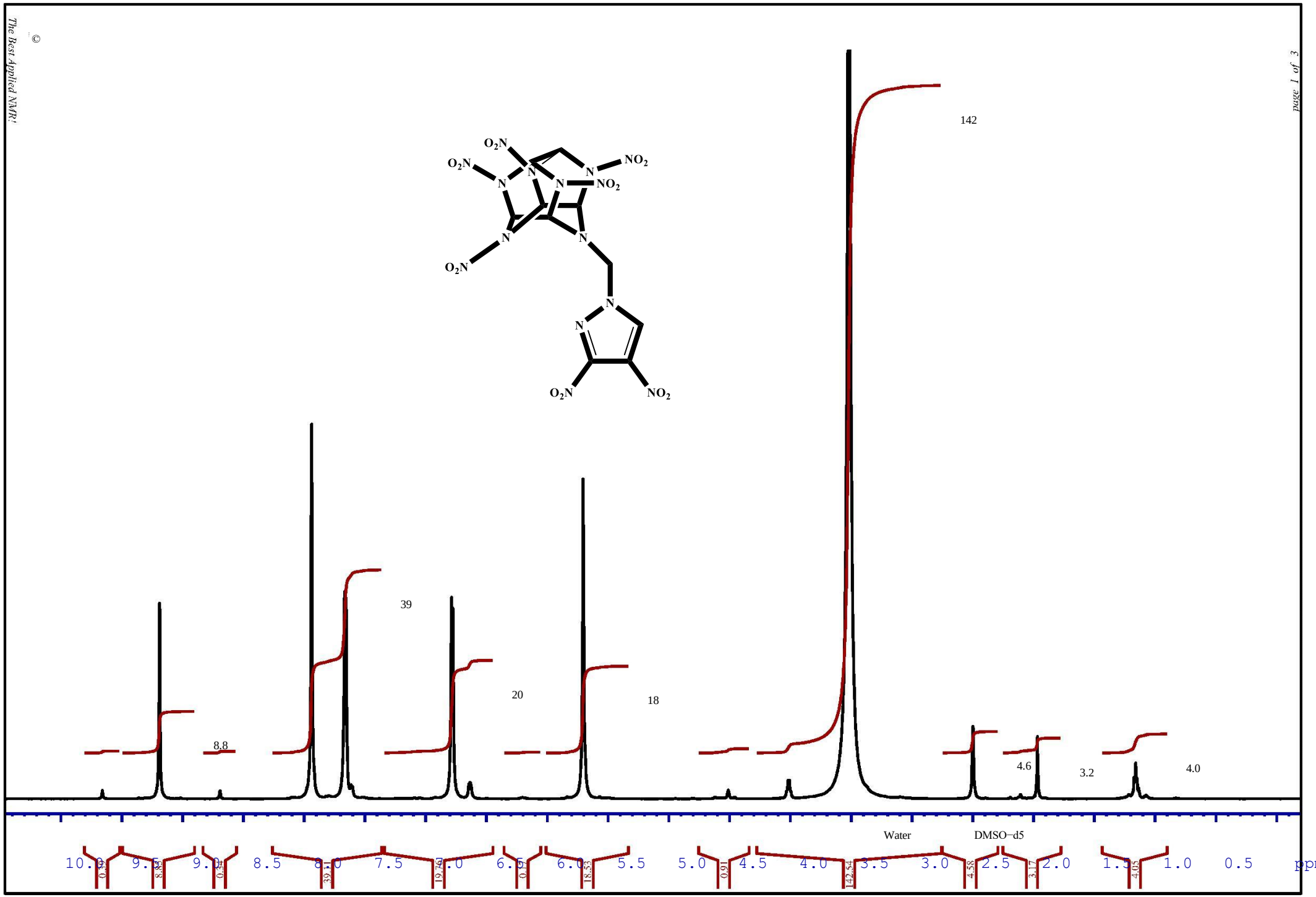
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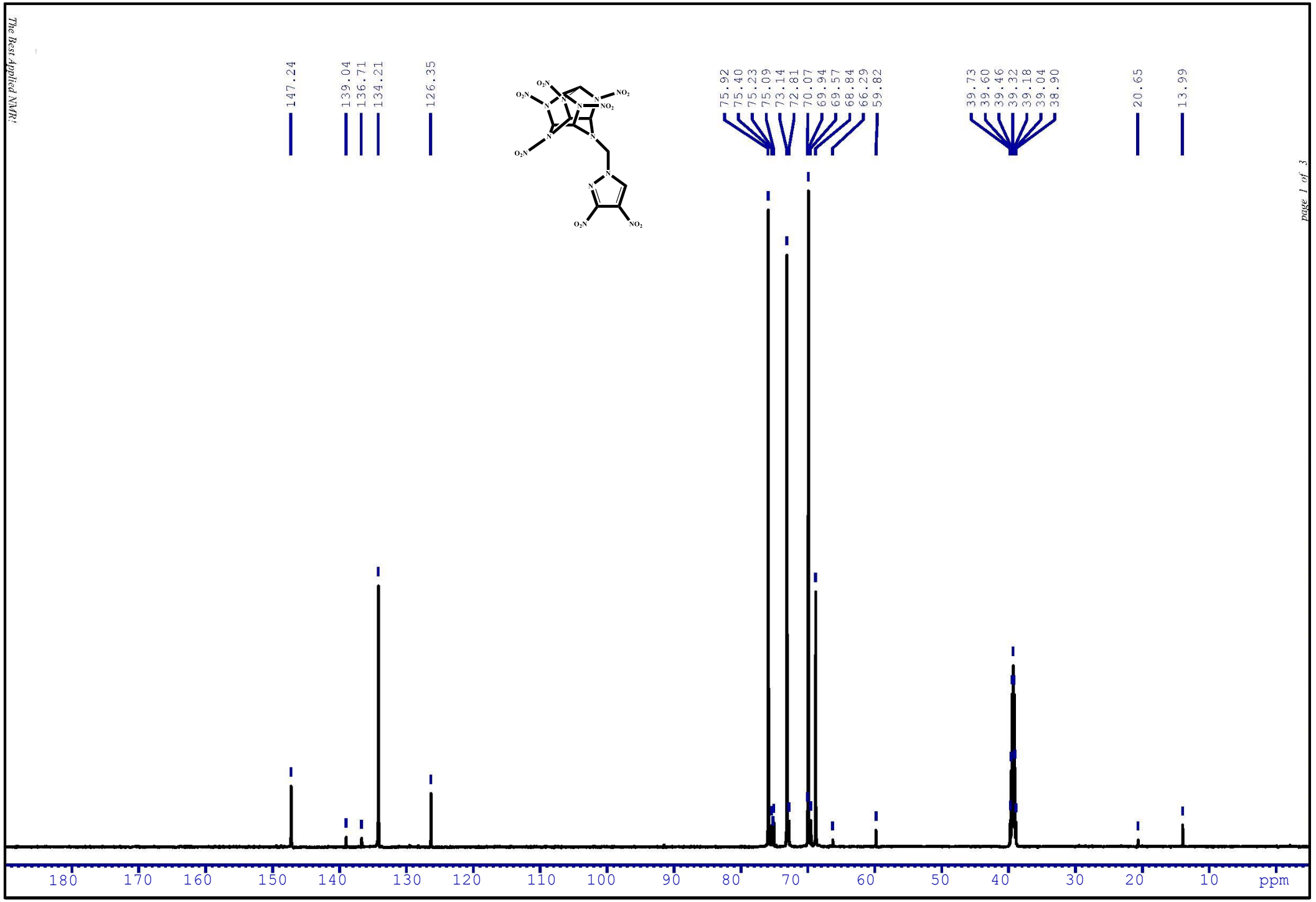
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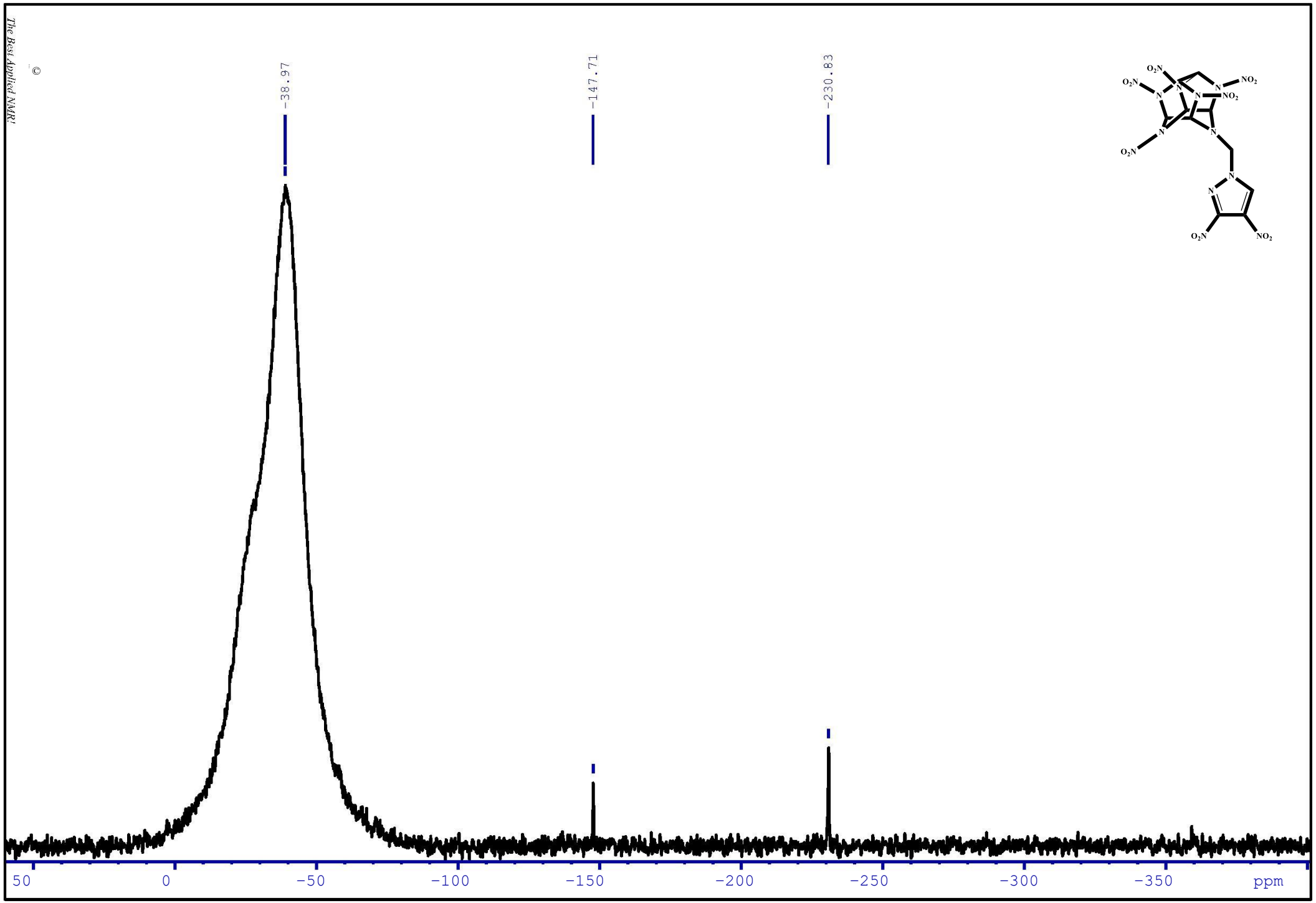
The Best Applied NMR!
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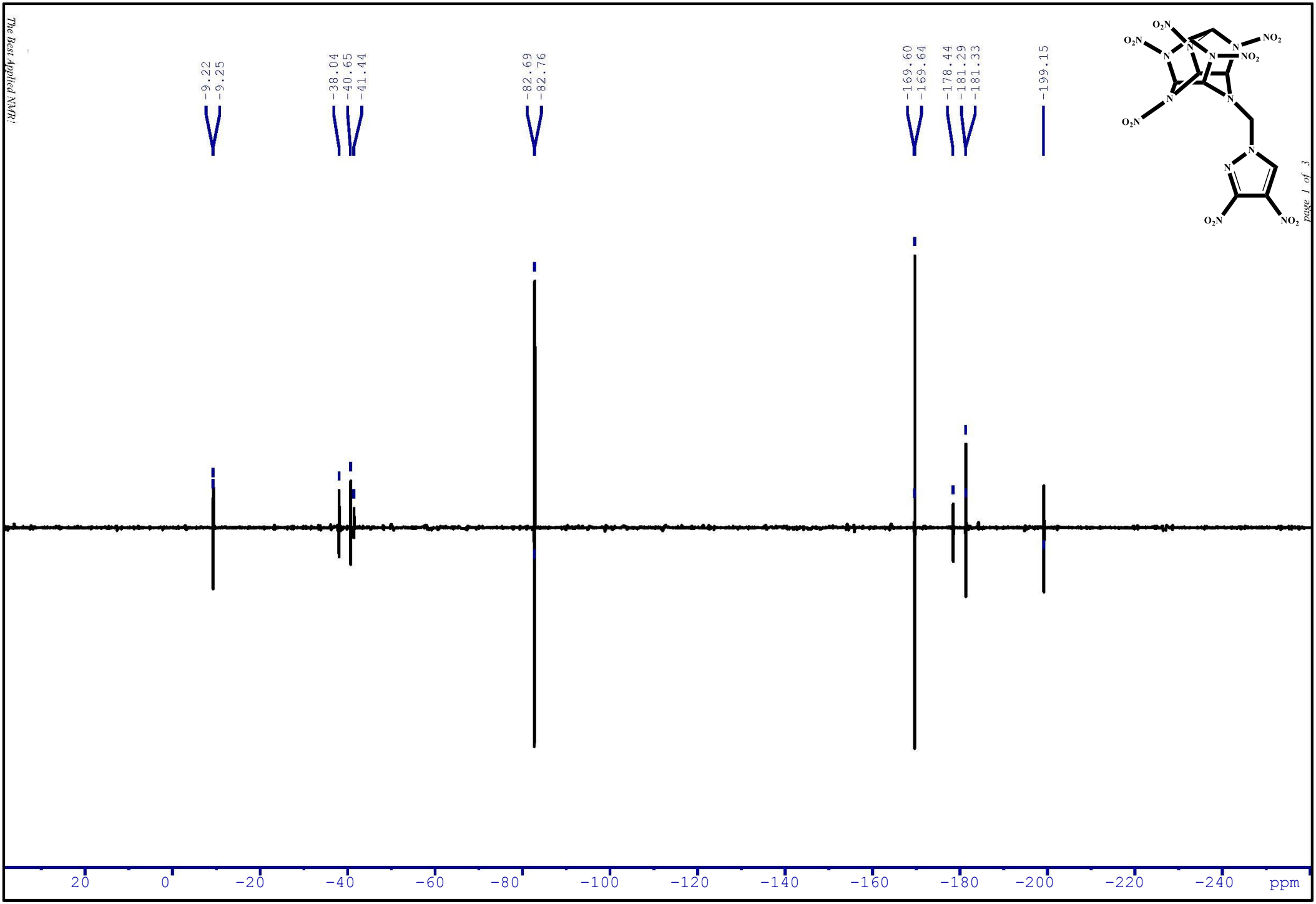
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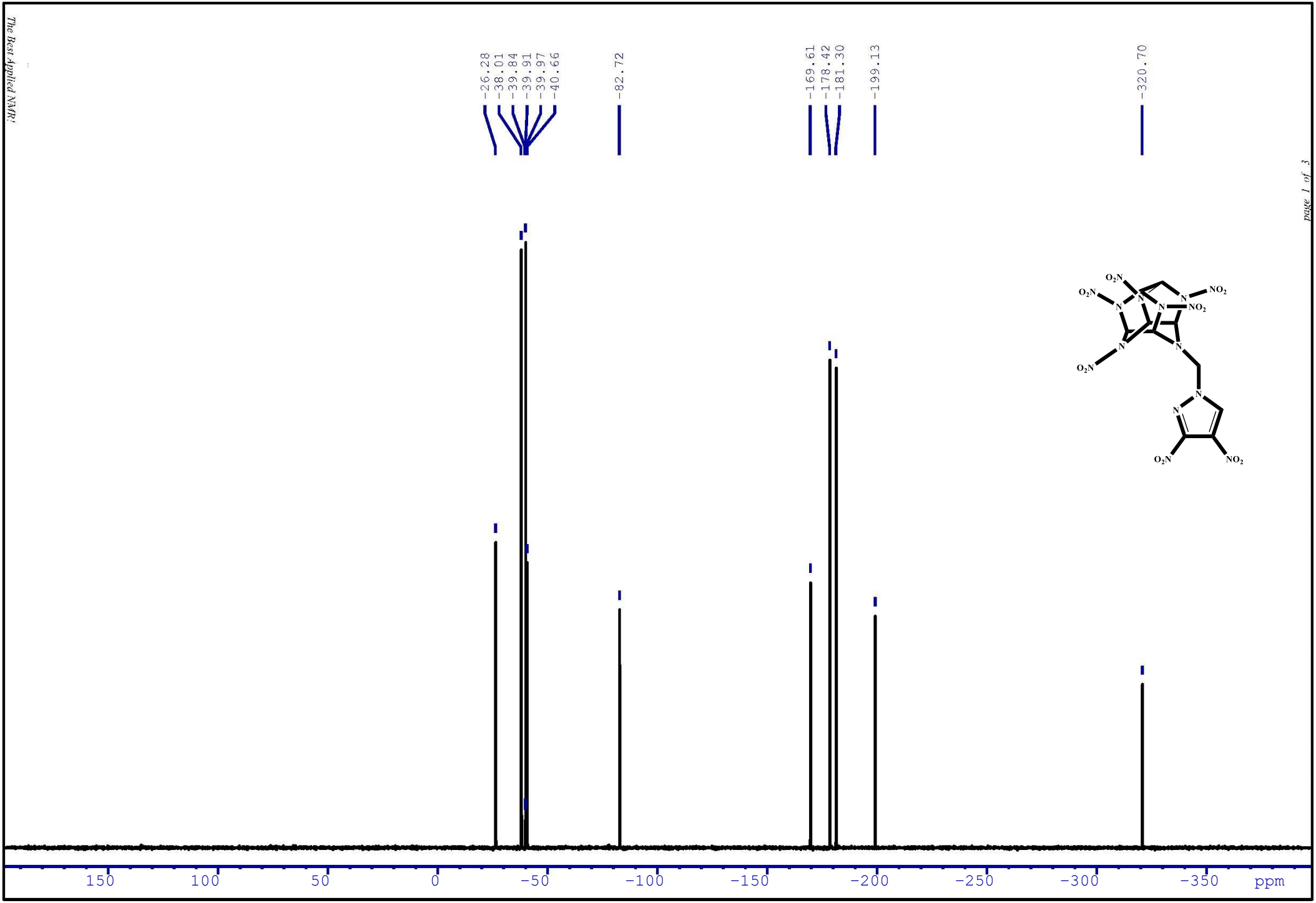
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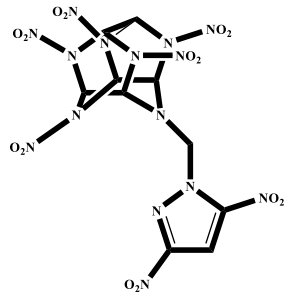

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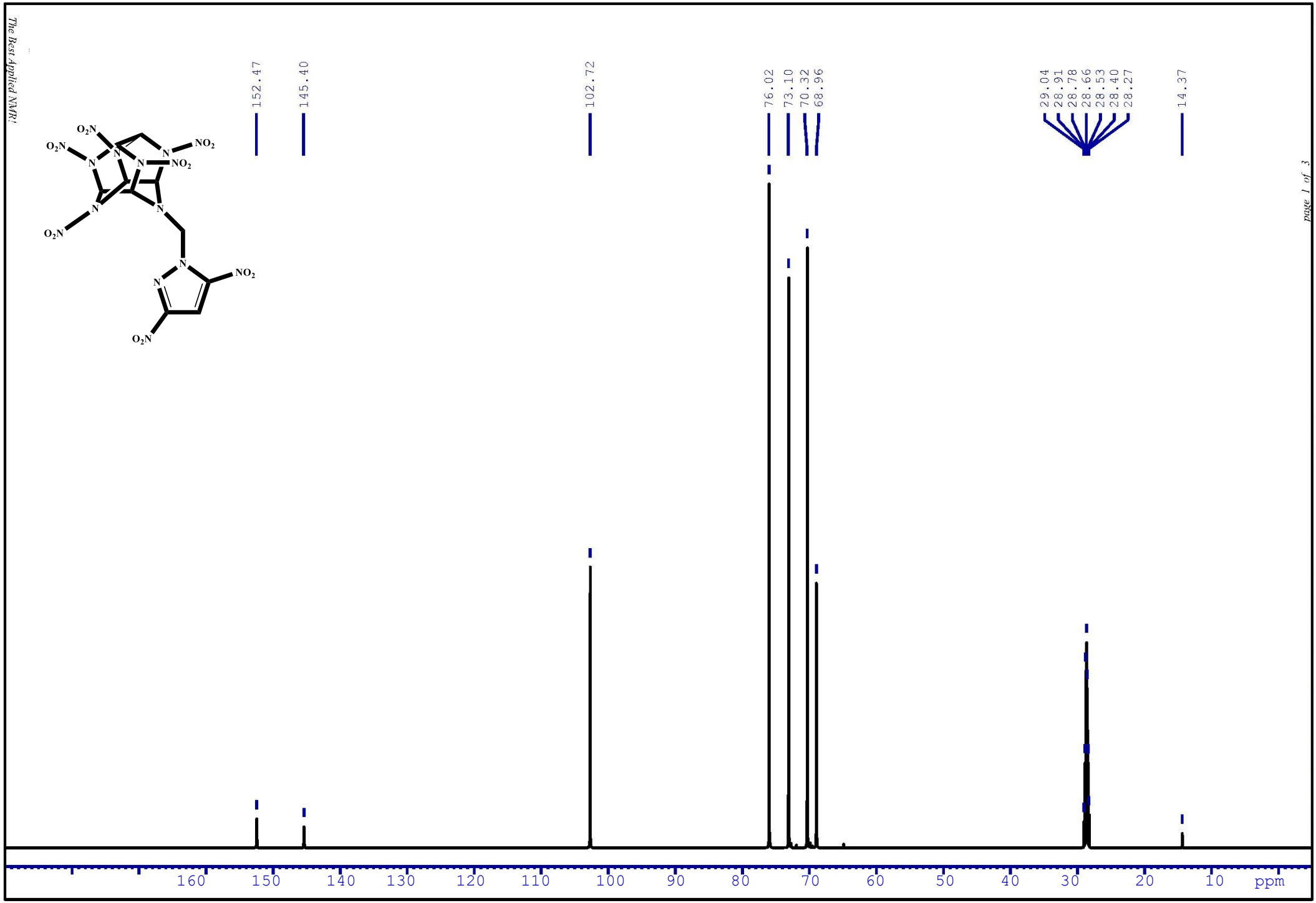
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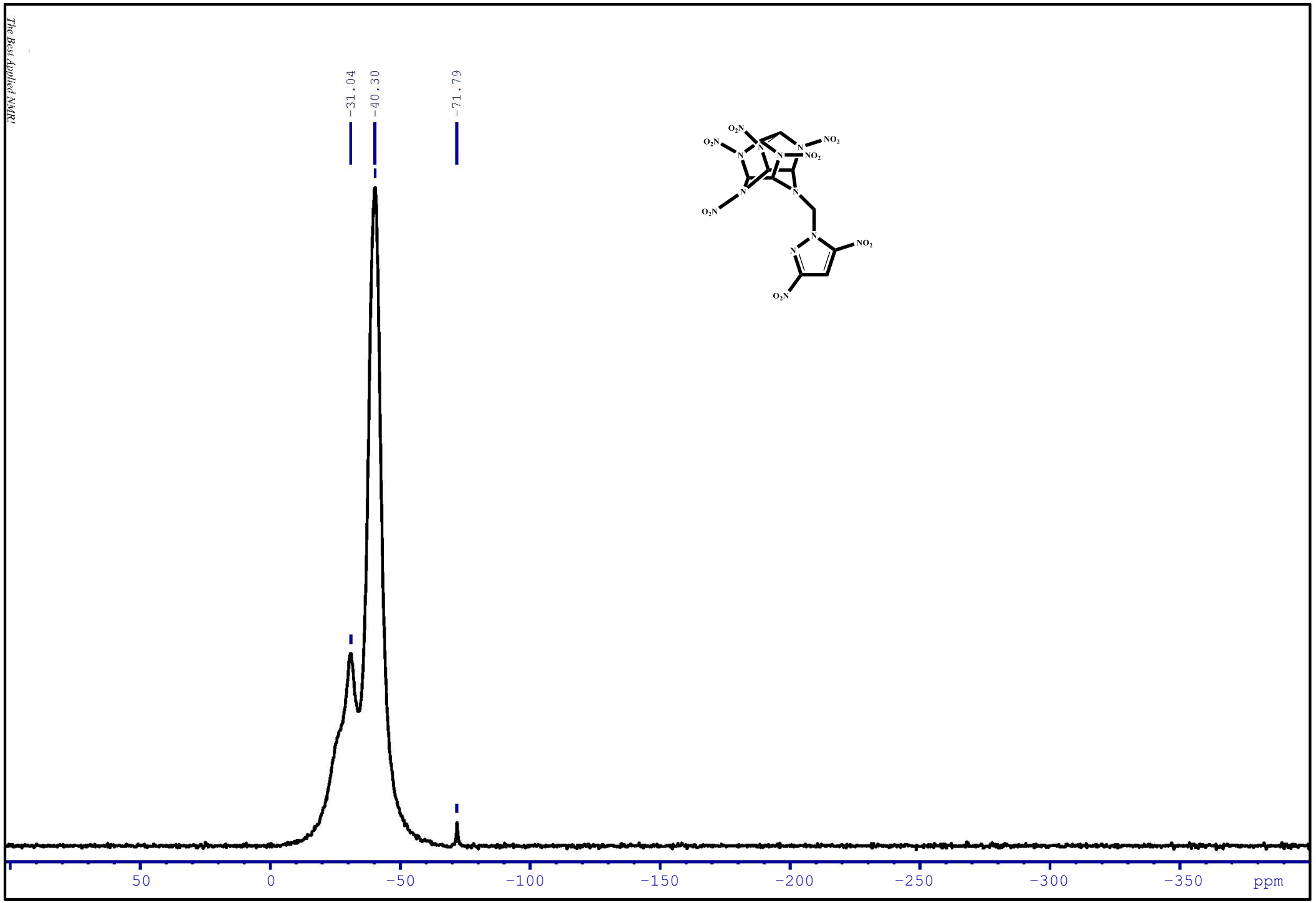
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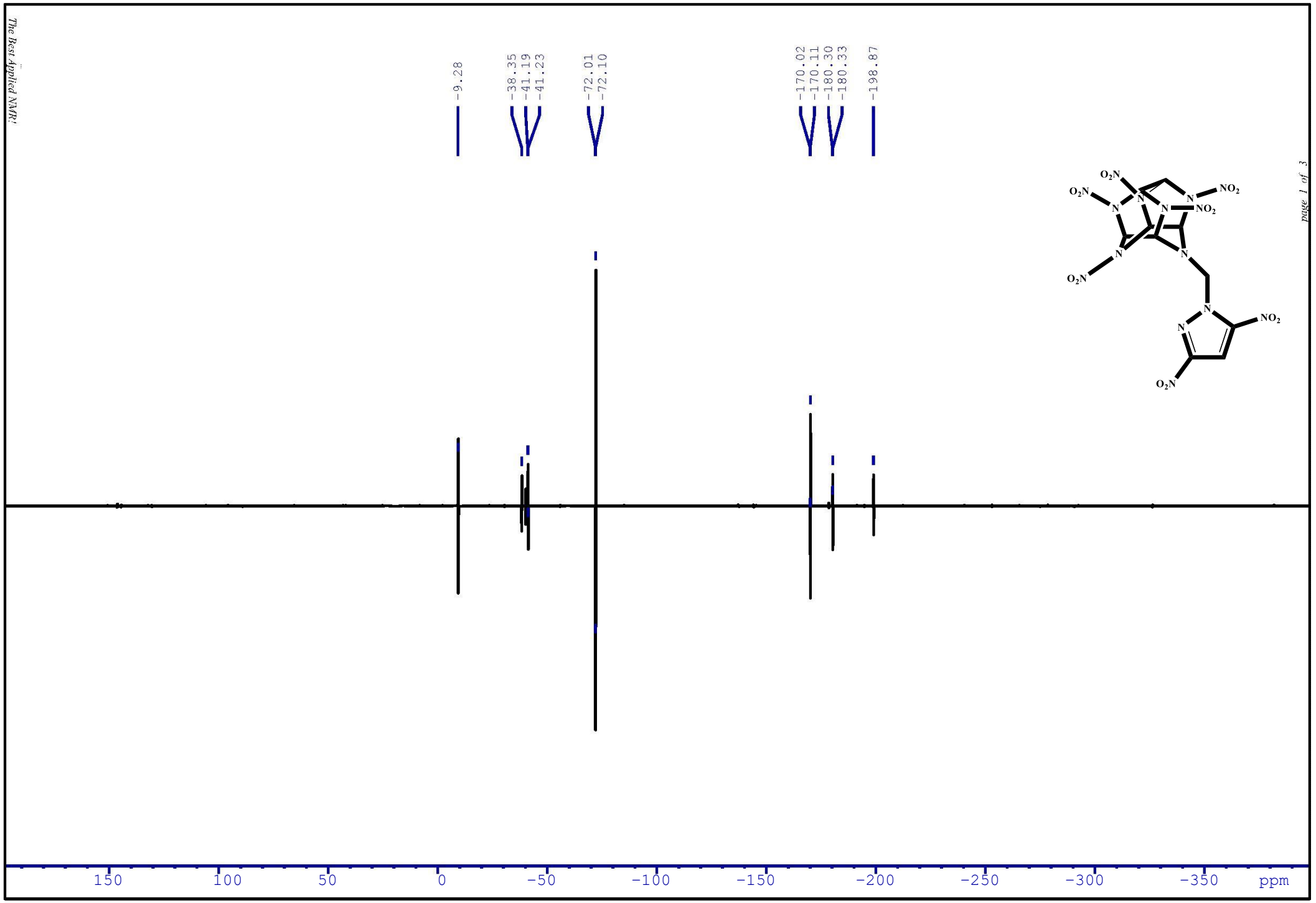
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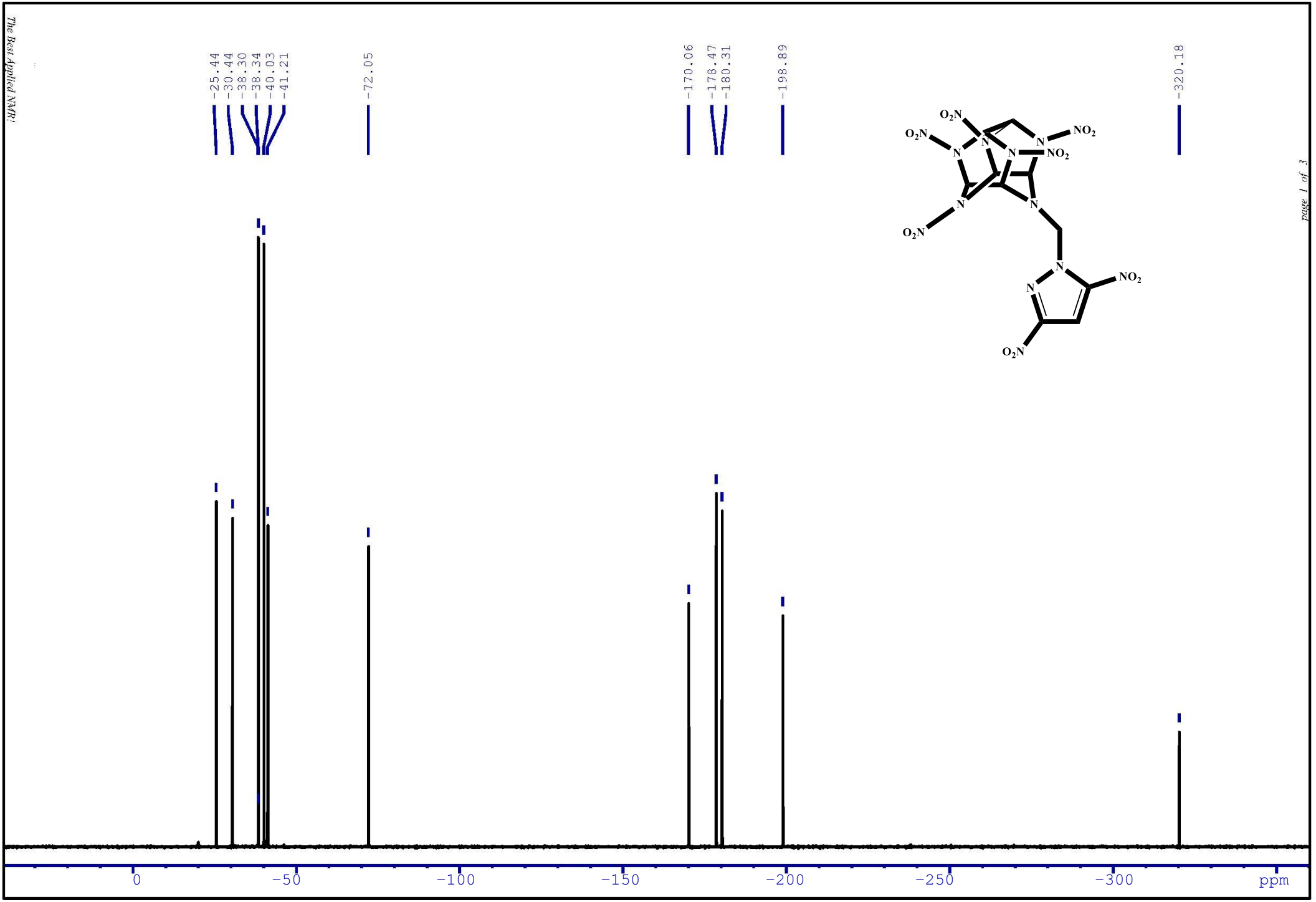
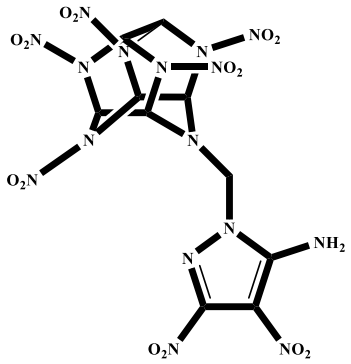
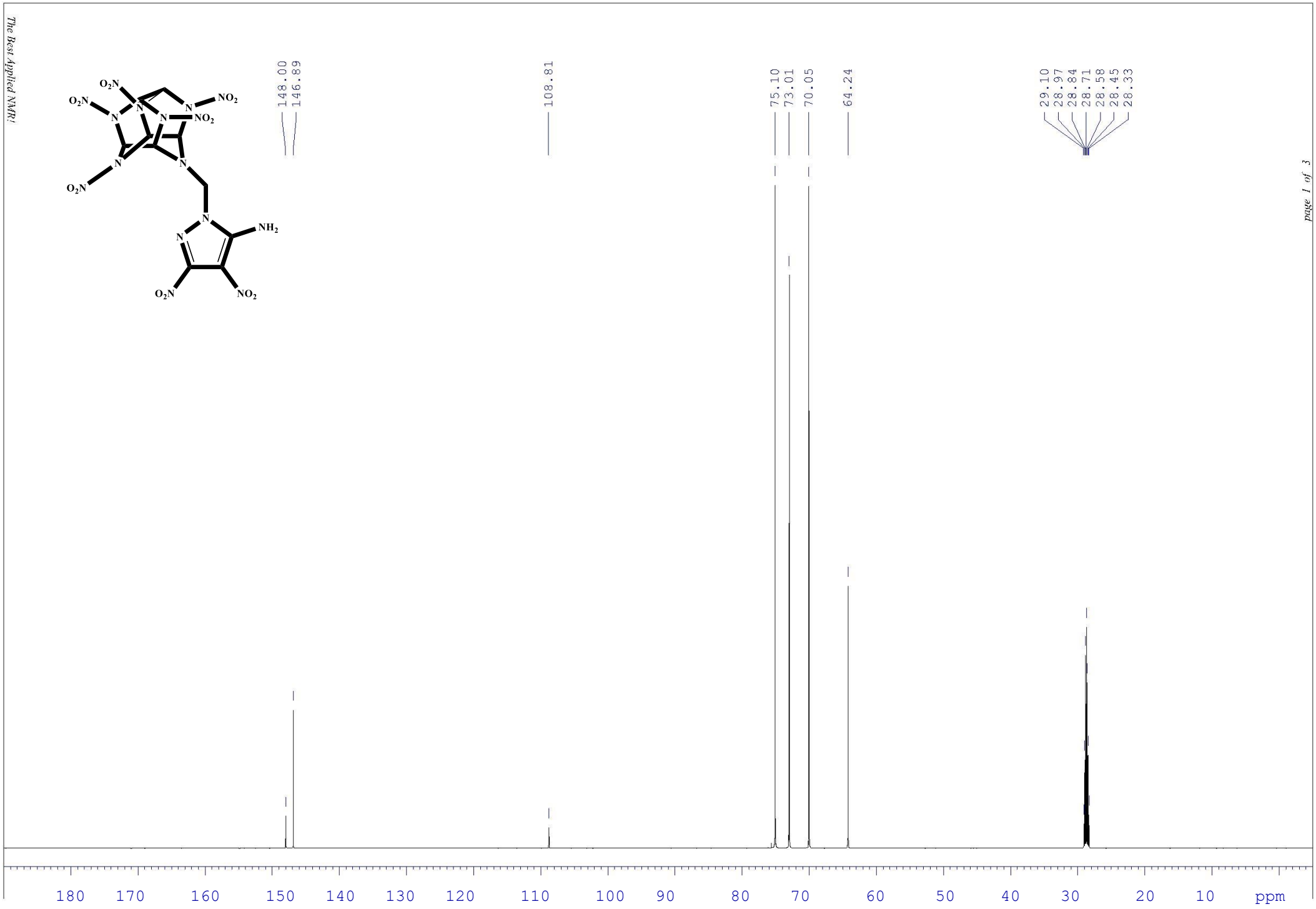
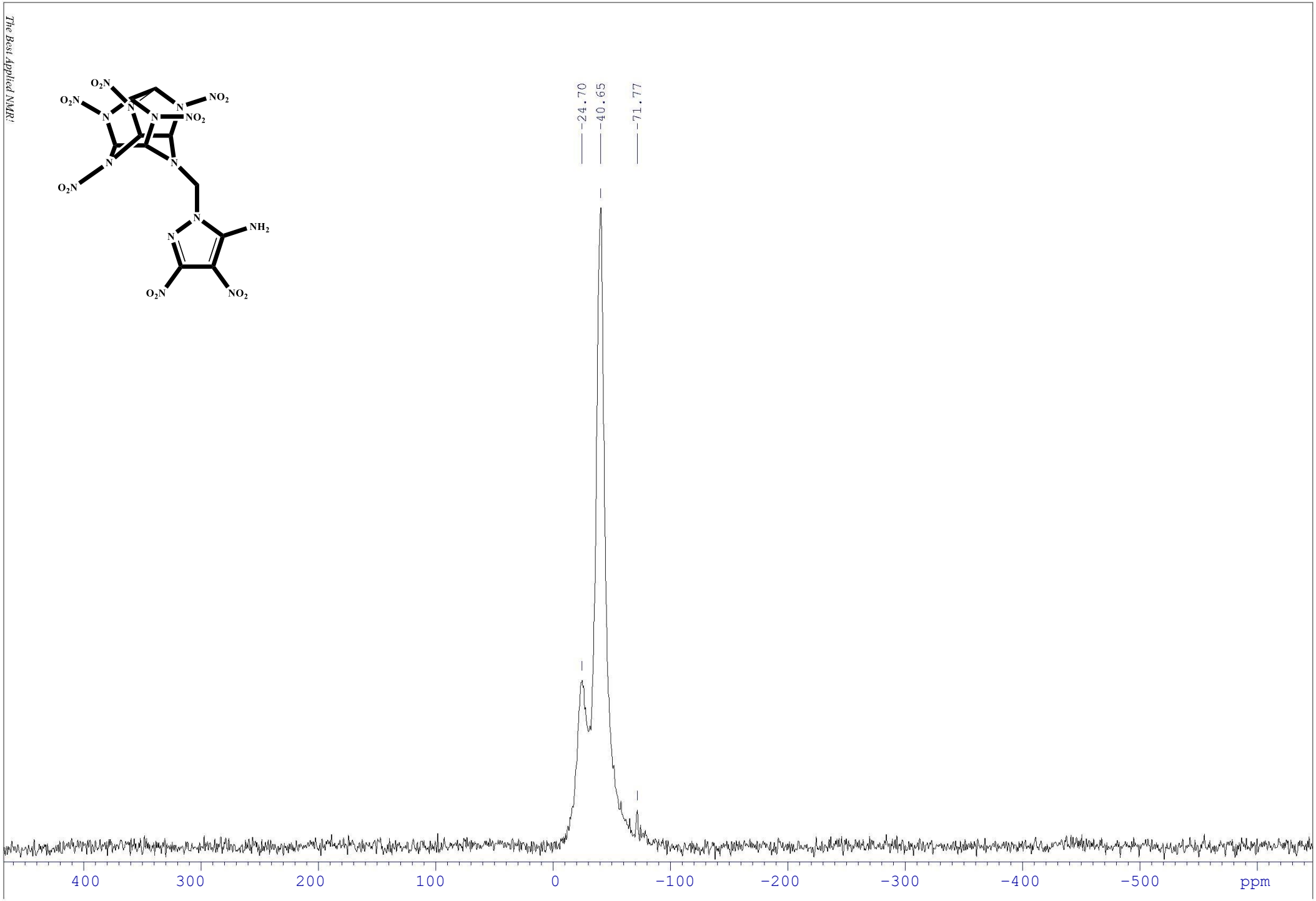
-180.30
-180.33
-198.87
page 1 of 3
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
ppm

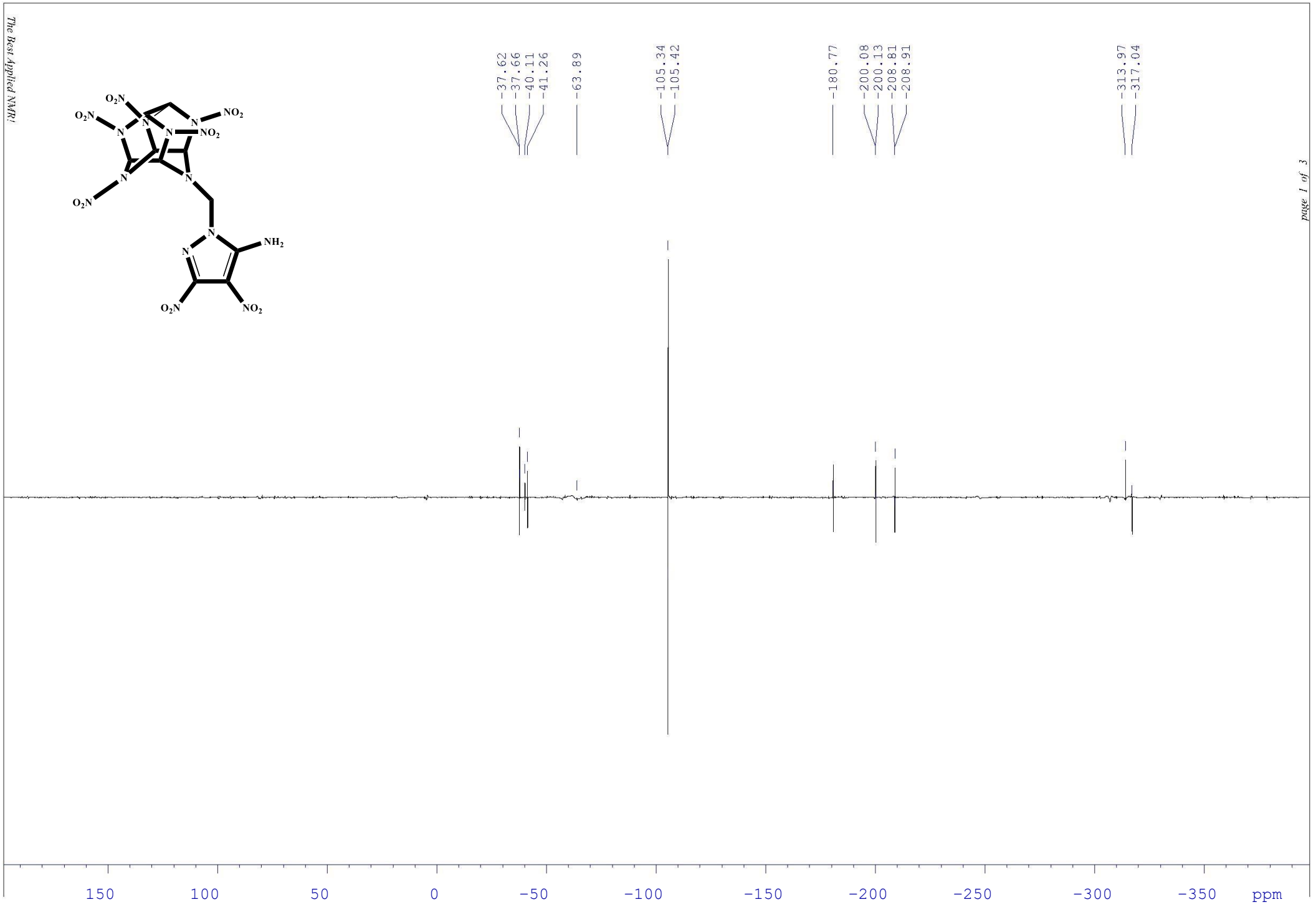

The Best Applied NMR!
-25.44
-30.44
-38.30
-38.34
-40.03
-41.21
-72.05
-170.06
-178.47
-180.31
-198.89
-320.18
page 1 of 3
0
-50
-100
-150
-200
-250
-300
ppm

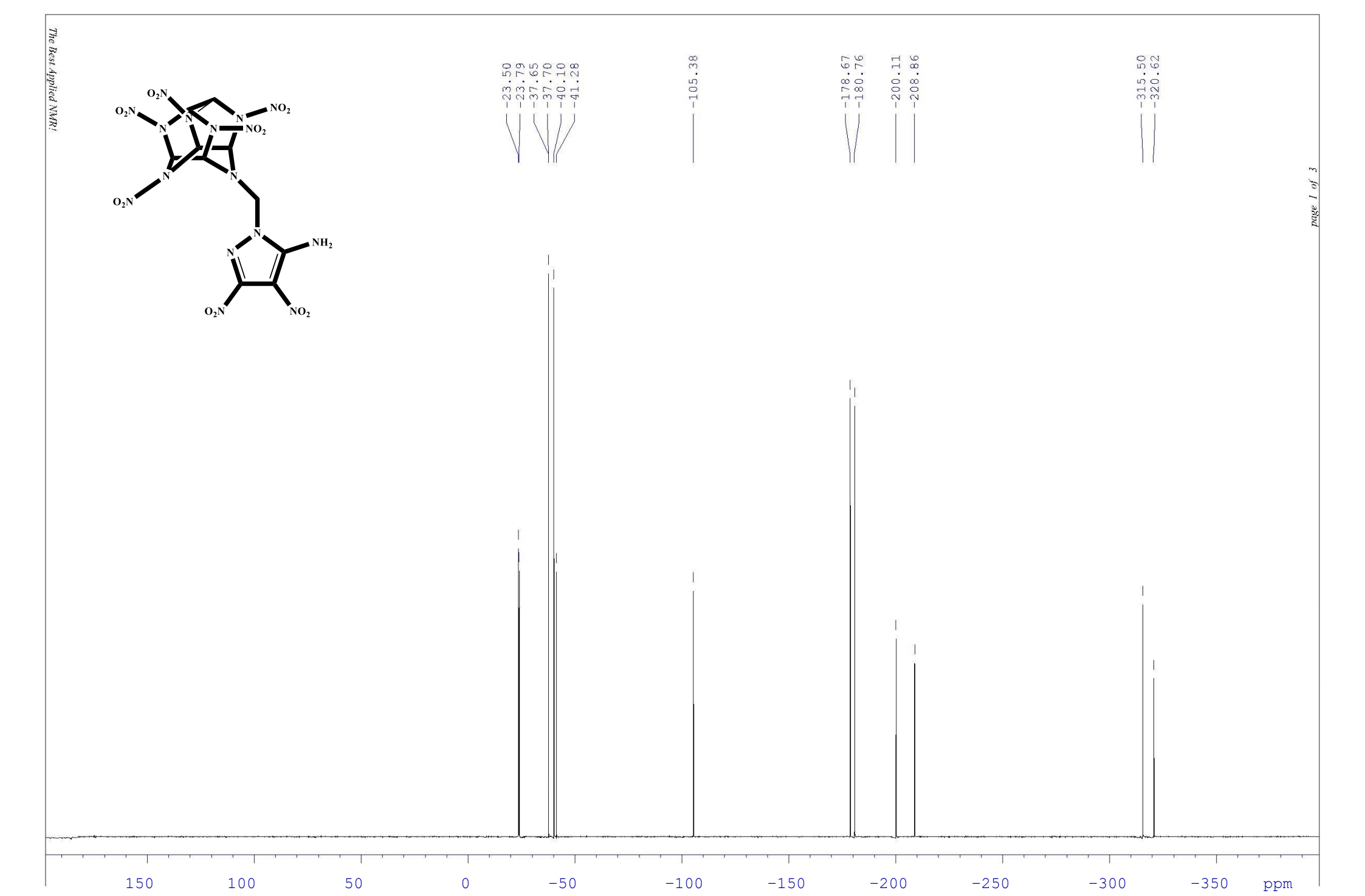

O2N
O2N
NO2
NO2
O2N
NH2
O2N
NO2

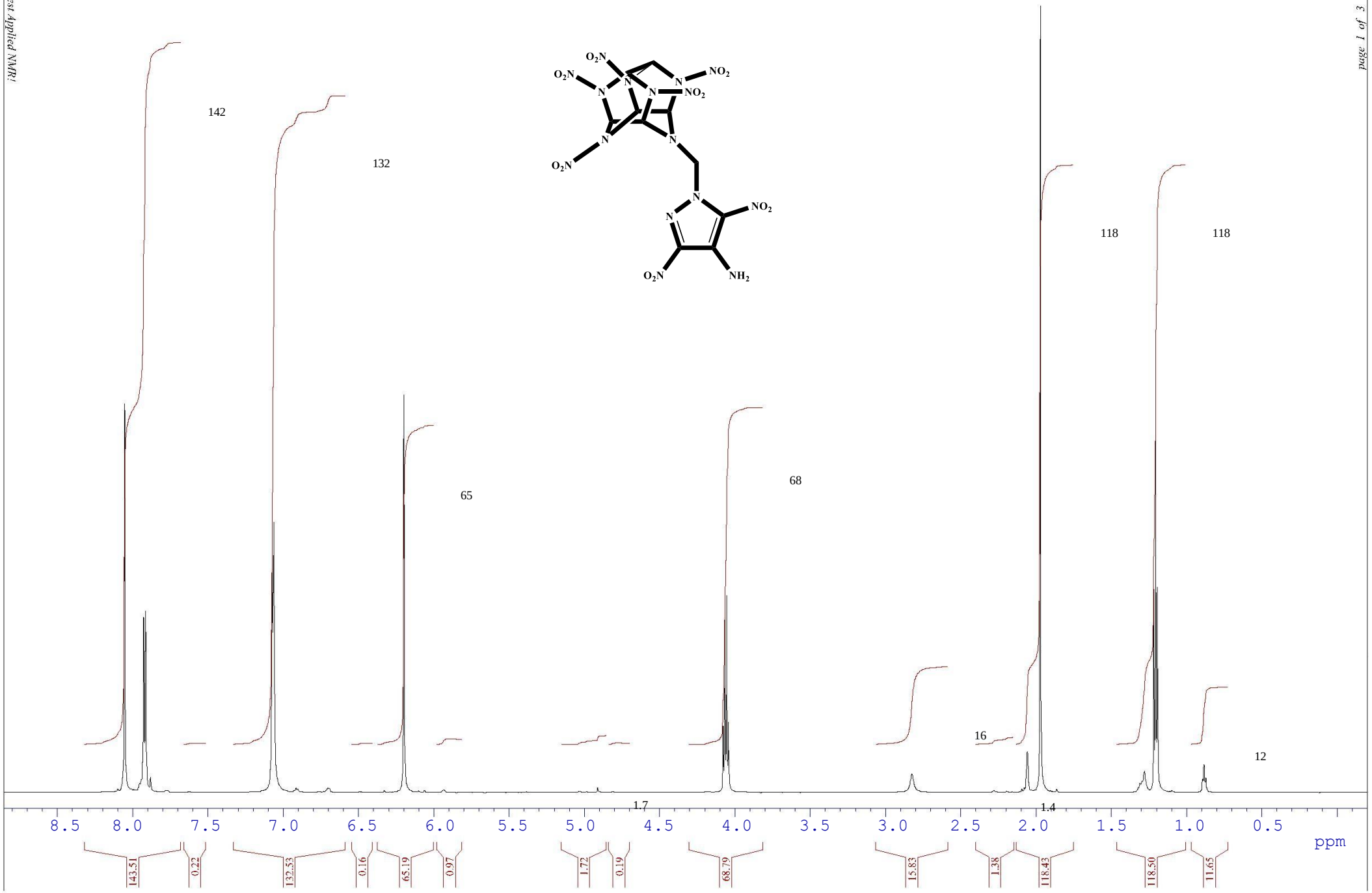
142
85
28
28
5.2
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
85.98
28.51
0.23
28.07
0.20
0.29
142.61
0.67
5.31
0.37
0.45

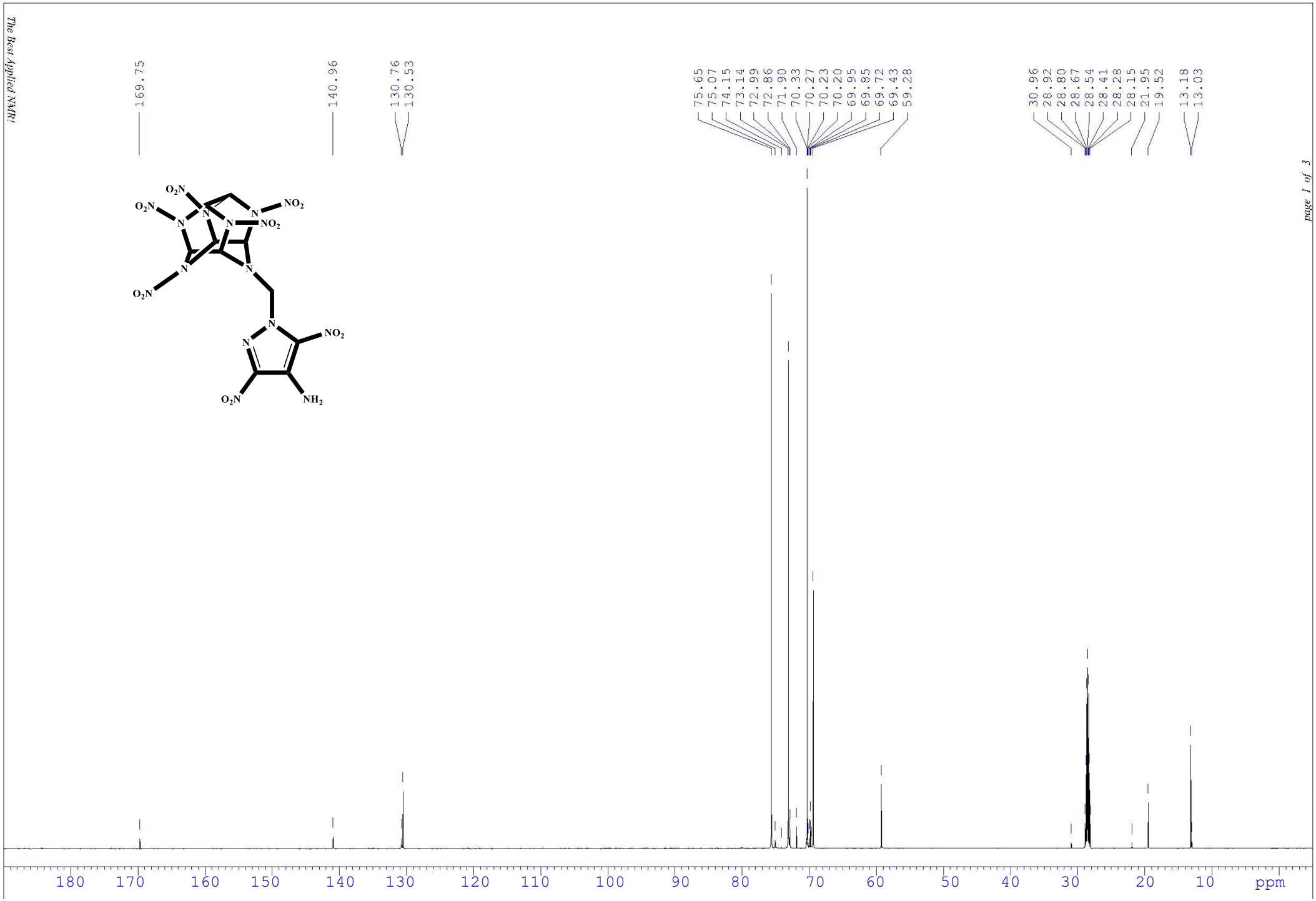

The Best Applied NMR!
148.00
146.89
108.81
75.10
73.01
70.05
64.24
29.10
28.97
28.84
28.71
28.58
28.45
28.33
page 1 of 3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

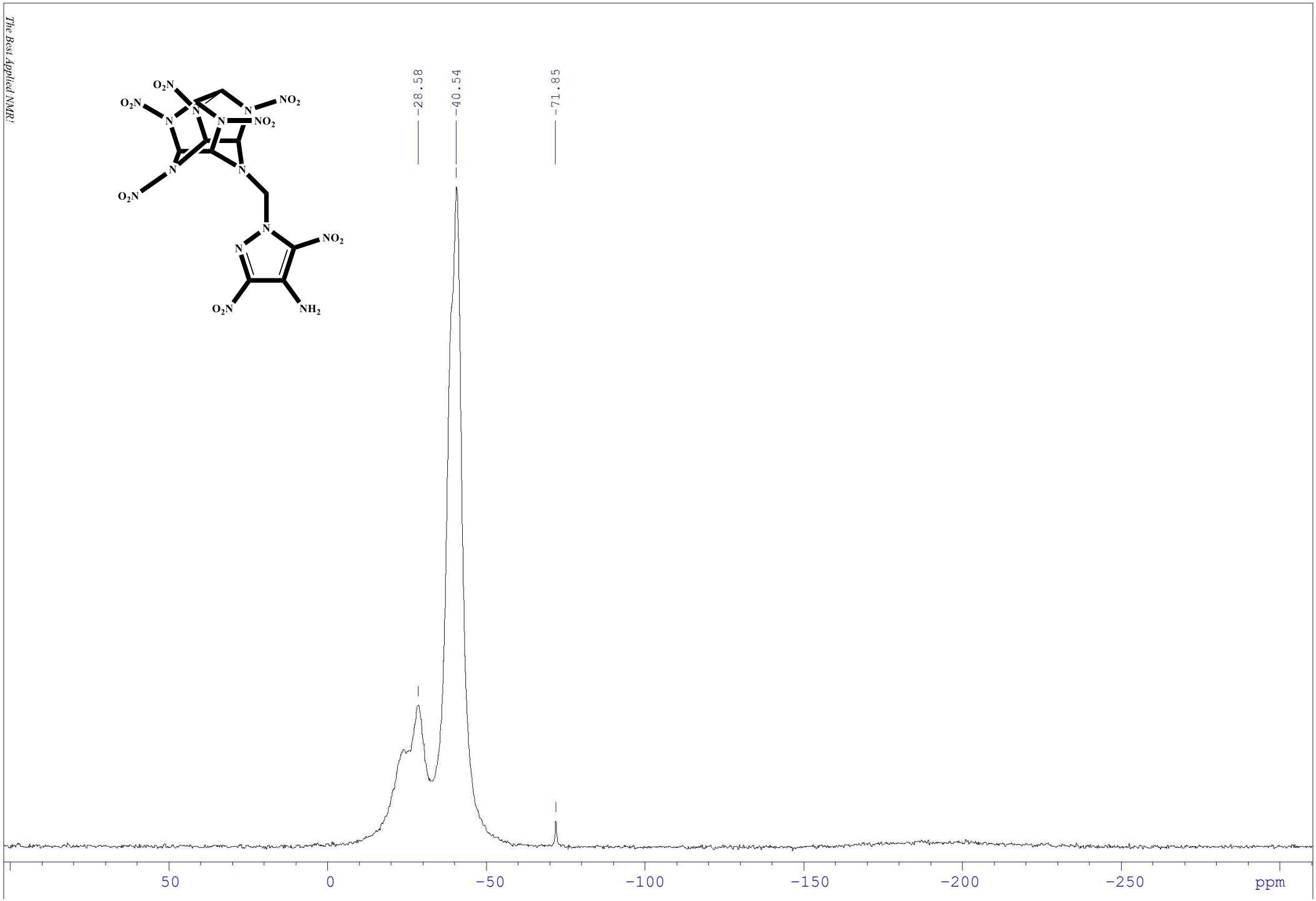

-24.70
-40.65
-71.77
400
300
200
100
0
-100
-200
-300
-400
-500
ppm

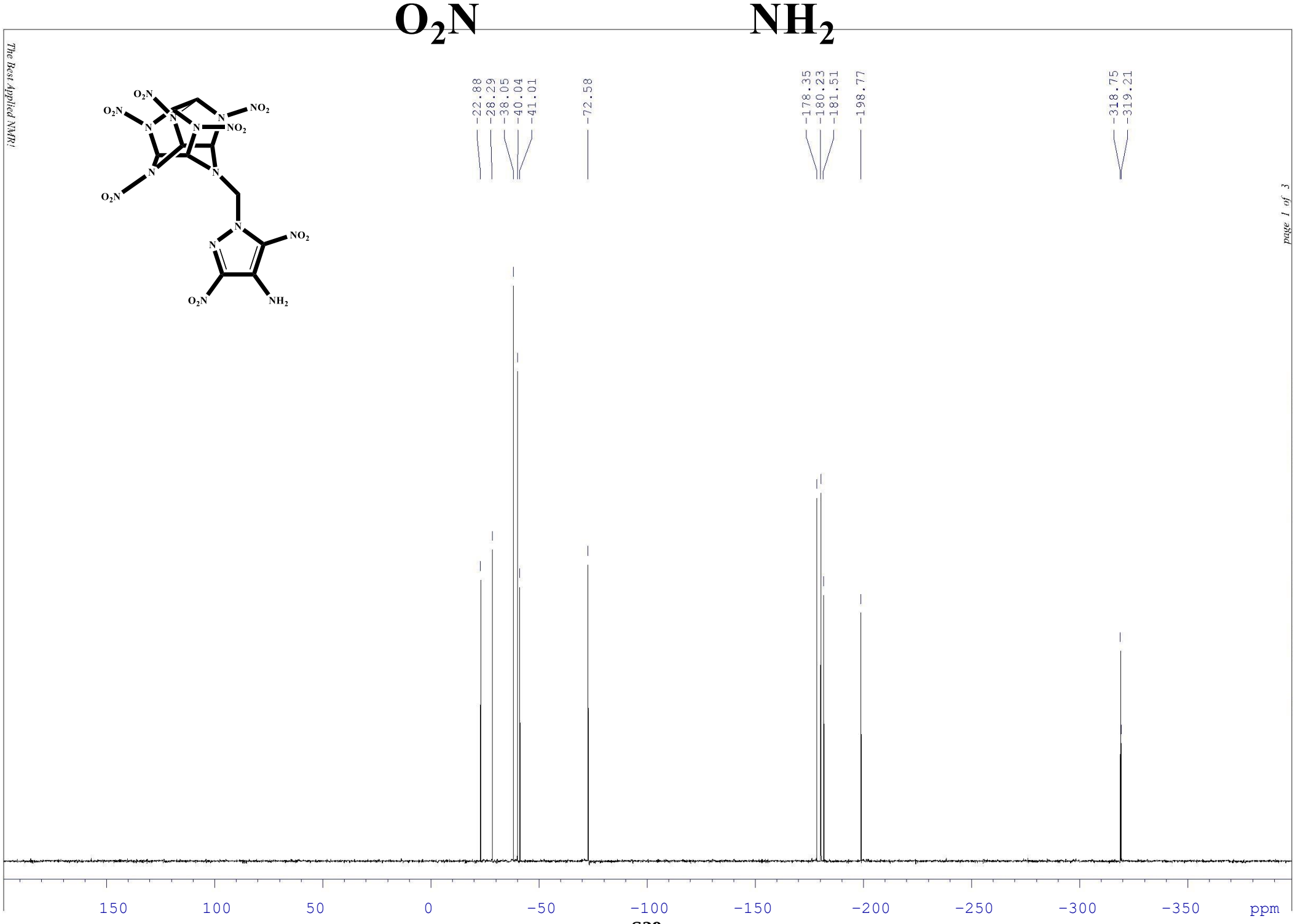

The Best Applied NMR!
-37.62
-37.66
-40.11
-41.26
-63.89
-105.34
-105.42
-180.77
-200.08
-200.13
-208.81
-208.91
-313.97
-317.04
page 1 of 3
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
ppm

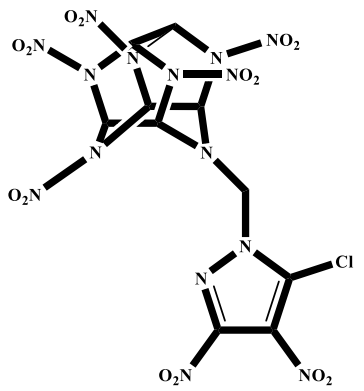

The Best Applied NMR!
-23.50
-23.79
-37.65
-37.70
-40.10
-41.28
-105.38
-178.67
-180.76
-200.11
-208.86
-315.50
-320.62
page 1 of 3
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
ppm


142
132
65
68
16
118
118
12
1.7
1.4
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm
143.51
0.22
132.53
0.16
65.19
0.97
1.72
0.19
68.79
15.83
1.38
118.43
118.50
11.65

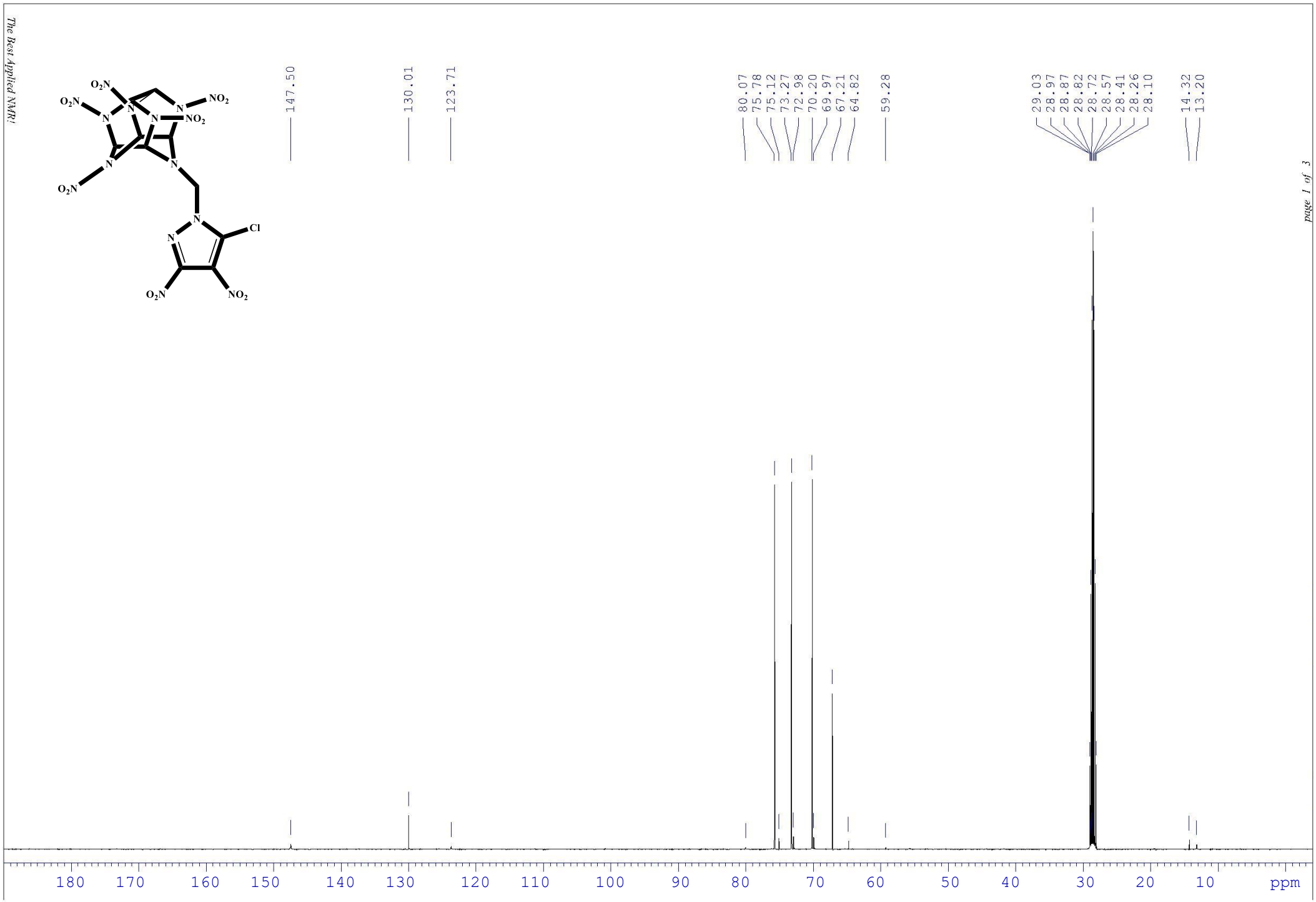

The Best Applied NMR!
169.75
140.96
130.76
130.53
75.65
75.07
74.15
73.14
72.99
72.86
71.90
70.33
70.27
70.23
70.20
69.95
69.85
69.72
69.43
59.28
30.96
28.92
28.80
28.67
28.54
28.41
28.28
28.15
21.95
19.52
13.18
13.03
page 1 of 3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

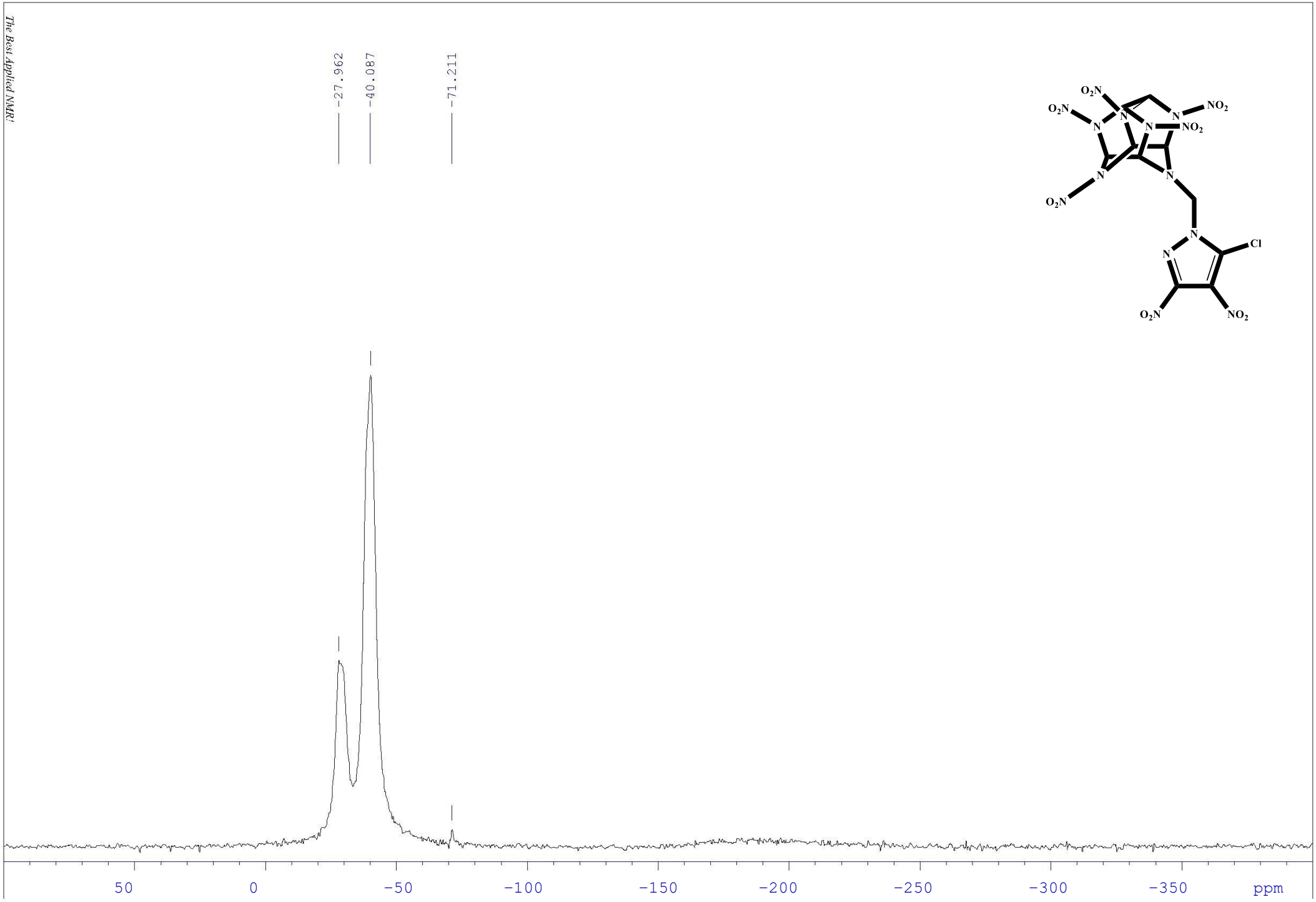

The Best Applied NMR!
-28.58
-40.54
-71.85
50
0
-50
-100
-150
-200
-250
ppm


O2N
NH2
The Best Applied NMR!
-22.88
-28.29
-38.05
-40.04
-41.01
-72.58
-178.35
-180.23
-181.51
-198.77
-318.75
-319.21
page 1 of 3
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
ppm


O2N
NO2
Cl

The Best Applied NMR!
142
67
67
71
24
16
11
4.8
3.3
3.6
1.4
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 ppm
0.12 0.34 34.14 0.05 0.18 0.13 16.18 0.87 0.05 0.14 16.10 −0.02 0.04 0.79 1.16 2.62 3.76 0.11 0.01 16.99 0.11 0.13 5.85 0.05 0.09


The Best Applied NMR!
147.50
130.01
123.71
80.07
75.78
75.12
73.27
72.98
70.20
69.97
67.21
64.82
59.28
29.03
28.97
28.87
28.82
28.72
28.57
28.41
28.26
28.10
14.32
13.20
page 1 of 3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


The Best Applied NMR!
-27.962
-40.087
-71.211
O2N
NO2
Cl
50
0
-50
-100
-150
-200
-250
-300
-350
ppm

X-ray crystallographic data

Table S2. Crystal data and structure refinement for **10-(4-nitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4a**.

Empirical formula	C13 H16 N14 O13	
Formula weight	576.40	
Temperature	100.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.4288(2) Å	α= 88.255(2)°.
	b = 9.5788(2) Å	β= 77.164(2)°.
	c = 14.1442(3) Å	γ = 77.275(2)°.
Volume	1085.88(4) Å3	
Z	2	
Density (calculated)	1.763 g/cm3	
Absorption coefficient	1.391 mm-1	
F(000)	592	
Crystal size	0.26 x 0.11 x 0.05 mm3	
Theta range for data collection	3.205 to 80.050°.	
Index ranges	-10<=h<=10, -12<=k<=12, -16<=l<=18	
Reflections collected	28748	
Independent reflections	4692 [R(int) = 0.0273]	
Observed reflections	4443	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.387	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	4692 / 0 / 364	
Goodness-of-fit on F2	1.086	
Final R indices [I>2sigma(I)]	R1 = 0.0391, wR2 = 0.1103	
R indices (all data)	R1 = 0.0405, wR2 = 0.1115	
Extinction coefficient	0.0022(4)	
Largest diff. peak and hole	0.534 and -0.258 e.Å-3	

Table S3. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for **10-(4-nitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	8635(1)	11054(1)	5895(1)	23(1)
O(2)	6632(2)	11457(1)	7200(1)	27(1)
O(3)	6517(1)	8735(1)	4029(1)	25(1)
O(4)	4781(1)	7441(1)	4732(1)	25(1)
O(5)	4741(2)	10125(1)	8795(1)	36(1)
O(6)	7237(2)	9367(2)	9063(1)	38(1)

O(7)	11944(1)	8661(1)	6454(1)	26(1)
O(8)	11004(2)	8170(2)	7954(1)	35(1)
O(9)	12071(1)	5486(1)	5410(1)	23(1)
O(10)	10732(1)	3999(1)	6261(1)	24(1)
O(11)	3911(2)	3447(2)	10401(1)	36(1)
O(12)	1352(2)	3665(2)	10253(1)	36(1)
N(1)	6842(1)	9634(1)	6220(1)	17(1)
N(2)	6846(1)	7652(1)	5433(1)	17(1)
N(3)	6575(2)	8475(1)	7798(1)	20(1)
N(4)	6460(2)	6281(1)	6906(1)	19(1)
N(5)	9379(2)	8247(1)	6888(1)	18(1)
N(6)	9325(1)	6218(1)	6069(1)	17(1)
N(7)	7411(2)	10784(1)	6461(1)	20(1)
N(8)	5969(2)	7992(1)	4683(1)	20(1)
N(9)	6151(2)	9407(2)	8612(1)	28(1)
N(10)	10899(2)	8333(1)	7116(1)	23(1)
N(11)	10841(2)	5167(1)	5918(1)	18(1)
N(12)	4636(2)	4726(1)	7573(1)	21(1)
N(13)	3010(2)	5072(2)	7499(1)	31(1)
N(14)	2815(2)	3752(2)	9932(1)	28(1)
C(1)	7968(2)	8572(1)	5514(1)	16(1)
C(2)	5818(2)	8914(2)	6988(1)	18(1)
C(3)	5787(2)	7532(2)	6426(1)	18(1)
C(4)	9496(2)	7696(1)	5914(1)	16(1)
C(5)	8213(2)	7558(2)	7582(1)	19(1)
C(6)	8124(2)	6186(2)	7021(1)	18(1)
C(7)	5948(2)	4969(2)	6754(1)	21(1)
C(8)	4825(2)	4230(2)	8445(1)	24(1)
C(9)	3242(2)	4227(2)	8962(1)	25(1)
C(10)	2163(2)	4753(2)	8349(1)	32(1)
O(31)	8572(2)	3649(2)	8566(1)	40(1)
C(31)	10799(4)	1616(3)	8354(2)	63(1)
C(32)	9217(2)	2531(2)	8894(1)	35(1)
C(33)	8452(3)	2051(2)	9877(2)	50(1)

Table S4. Bond lengths [Å] and angles [°] for **10-(4-nitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4a**.

O(1)-N(7)	1.2284(16)
O(2)-N(7)	1.2201(17)
O(3)-N(8)	1.2202(17)
O(4)-N(8)	1.2189(17)
O(5)-N(9)	1.2112(19)
O(6)-N(9)	1.220(2)
O(7)-N(10)	1.2207(17)
O(8)-N(10)	1.2113(18)
O(9)-N(11)	1.2167(16)
O(10)-N(11)	1.2198(16)
O(11)-N(14)	1.2323(19)

O(12)-N(14)	1.2361(19)
N(1)-N(7)	1.3746(17)
N(1)-C(1)	1.4650(17)
N(1)-C(2)	1.4844(17)
N(2)-N(8)	1.4146(17)
N(2)-C(1)	1.4504(17)
N(2)-C(3)	1.5042(17)
N(3)-N(9)	1.4110(18)
N(3)-C(2)	1.4395(19)
N(3)-C(5)	1.4377(18)
N(4)-C(3)	1.4277(18)
N(4)-C(6)	1.4300(18)
N(4)-C(7)	1.4525(18)
N(5)-N(10)	1.4085(17)
N(5)-C(4)	1.4642(17)
N(5)-C(5)	1.4773(17)
N(6)-N(11)	1.4201(16)
N(6)-C(4)	1.4597(17)
N(6)-C(6)	1.4981(17)
N(12)-N(13)	1.3643(19)
N(12)-C(7)	1.4649(18)
N(12)-C(8)	1.339(2)
N(13)-C(10)	1.320(2)
N(14)-C(9)	1.427(2)
C(1)-H(1)	1.0000
C(1)-C(4)	1.5817(18)
C(2)-H(2)	1.0000
C(2)-C(3)	1.572(2)
C(3)-H(3)	1.0000
C(4)-H(4)	1.0000
C(5)-H(5)	1.0000
C(5)-C(6)	1.580(2)
C(6)-H(6)	1.0000
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8)	0.9500
C(8)-C(9)	1.372(2)
C(9)-C(10)	1.397(2)
C(10)-H(10)	0.9500
O(31)-C(32)	1.218(2)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(31)-C(32)	1.483(3)
C(32)-C(33)	1.502(3)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
N(7)-N(1)-C(1)	118.53(11)
N(7)-N(1)-C(2)	119.57(11)
C(1)-N(1)-C(2)	110.01(10)

N(8)-N(2)-C(1)	115.36(11)
N(8)-N(2)-C(3)	115.50(11)
C(1)-N(2)-C(3)	107.95(10)
N(9)-N(3)-C(2)	118.33(12)
N(9)-N(3)-C(5)	117.92(12)
C(5)-N(3)-C(2)	116.72(11)
C(3)-N(4)-C(6)	114.84(11)
C(3)-N(4)-C(7)	117.64(12)
C(6)-N(4)-C(7)	118.59(12)
N(10)-N(5)-C(4)	115.93(11)
N(10)-N(5)-C(5)	118.57(11)
C(4)-N(5)-C(5)	107.91(11)
N(11)-N(6)-C(4)	115.69(11)
N(11)-N(6)-C(6)	116.37(10)
C(4)-N(6)-C(6)	107.27(10)
O(1)-N(7)-N(1)	116.48(12)
O(2)-N(7)-O(1)	126.41(13)
O(2)-N(7)-N(1)	117.08(12)
O(3)-N(8)-N(2)	117.61(12)
O(4)-N(8)-O(3)	126.43(13)
O(4)-N(8)-N(2)	115.82(12)
O(5)-N(9)-O(6)	127.70(14)
O(5)-N(9)-N(3)	116.18(14)
O(6)-N(9)-N(3)	116.10(13)
O(7)-N(10)-N(5)	116.00(12)
O(8)-N(10)-O(7)	126.37(13)
O(8)-N(10)-N(5)	117.45(13)
O(9)-N(11)-O(10)	126.90(12)
O(9)-N(11)-N(6)	117.38(11)
O(10)-N(11)-N(6)	115.49(11)
N(13)-N(12)-C(7)	119.73(12)
C(8)-N(12)-N(13)	113.07(12)
C(8)-N(12)-C(7)	127.16(13)
C(10)-N(13)-N(12)	104.63(13)
O(11)-N(14)-O(12)	123.76(14)
O(11)-N(14)-C(9)	118.83(14)
O(12)-N(14)-C(9)	117.41(14)
N(1)-C(1)-H(1)	111.4
N(1)-C(1)-C(4)	112.57(11)
N(2)-C(1)-N(1)	99.68(10)
N(2)-C(1)-H(1)	111.4
N(2)-C(1)-C(4)	109.95(10)
C(4)-C(1)-H(1)	111.4
N(1)-C(2)-H(2)	111.1
N(1)-C(2)-C(3)	101.05(10)
N(3)-C(2)-N(1)	113.82(12)
N(3)-C(2)-H(2)	111.1
N(3)-C(2)-C(3)	108.25(11)
C(3)-C(2)-H(2)	111.1
N(2)-C(3)-C(2)	104.28(10)
N(2)-C(3)-H(3)	110.2

N(4)-C(3)-N(2)	111.68(11)
N(4)-C(3)-C(2)	110.11(12)
N(4)-C(3)-H(3)	110.2
C(2)-C(3)-H(3)	110.2
N(5)-C(4)-C(1)	108.43(10)
N(5)-C(4)-H(4)	111.5
N(6)-C(4)-N(5)	104.19(10)
N(6)-C(4)-C(1)	109.34(11)
N(6)-C(4)-H(4)	111.5
C(1)-C(4)-H(4)	111.5
N(3)-C(5)-N(5)	110.39(11)
N(3)-C(5)-H(5)	111.2
N(3)-C(5)-C(6)	108.02(11)
N(5)-C(5)-H(5)	111.2
N(5)-C(5)-C(6)	104.70(11)
C(6)-C(5)-H(5)	111.2
N(4)-C(6)-N(6)	112.14(11)
N(4)-C(6)-C(5)	110.03(11)
N(4)-C(6)-H(6)	110.3
N(6)-C(6)-C(5)	103.57(10)
N(6)-C(6)-H(6)	110.3
C(5)-C(6)-H(6)	110.3
N(4)-C(7)-N(12)	110.60(11)
N(4)-C(7)-H(7A)	109.5
N(4)-C(7)-H(7B)	109.5
N(12)-C(7)-H(7A)	109.5
N(12)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
N(12)-C(8)-H(8)	127.4
N(12)-C(8)-C(9)	105.10(14)
C(9)-C(8)-H(8)	127.4
C(8)-C(9)-N(14)	125.67(15)
C(8)-C(9)-C(10)	106.76(14)
C(10)-C(9)-N(14)	127.56(15)
N(13)-C(10)-C(9)	110.42(15)
N(13)-C(10)-H(10)	124.8
C(9)-C(10)-H(10)	124.8
H(31A)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(32)-C(31)-H(31A)	109.5
C(32)-C(31)-H(31B)	109.5
C(32)-C(31)-H(31C)	109.5
O(31)-C(32)-C(31)	121.6(2)
O(31)-C(32)-C(33)	120.7(2)
C(31)-C(32)-C(33)	117.6(2)
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33C)	109.5

H(33B)-C(33)-H(33C) 109.5

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters (Å2x 103) for **10-(4-nitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4a**. The anisotropic displacement factor exponent takes the form: -2□2[h2 a*2U11 + .. + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	22(1)	22(1)	24(1)	6(1)	-1(1)	-9(1)
O(2)	32(1)	21(1)	24(1)	-4(1)	1(1)	-4(1)
O(3)	23(1)	29(1)	22(1)	8(1)	-7(1)	-4(1)
O(4)	21(1)	29(1)	29(1)	1(1)	-9(1)	-9(1)
O(5)	34(1)	35(1)	27(1)	-4(1)	6(1)	3(1)
O(6)	43(1)	43(1)	29(1)	-7(1)	-11(1)	-7(1)
O(7)	18(1)	30(1)	32(1)	5(1)	-5(1)	-8(1)
O(8)	37(1)	48(1)	27(1)	9(1)	-18(1)	-15(1)
O(9)	16(1)	24(1)	24(1)	1(1)	1(1)	-2(1)
O(10)	26(1)	17(1)	25(1)	5(1)	-1(1)	0(1)
O(11)	33(1)	50(1)	27(1)	12(1)	-11(1)	-12(1)
O(12)	26(1)	50(1)	30(1)	13(1)	1(1)	-11(1)
N(1)	15(1)	15(1)	18(1)	2(1)	0(1)	-3(1)
N(2)	14(1)	19(1)	17(1)	3(1)	-3(1)	-4(1)
N(3)	20(1)	21(1)	16(1)	1(1)	0(1)	-2(1)
N(4)	16(1)	16(1)	22(1)	5(1)	-2(1)	-5(1)
N(5)	16(1)	21(1)	16(1)	4(1)	-4(1)	-5(1)
N(6)	13(1)	16(1)	19(1)	4(1)	-1(1)	-1(1)
N(7)	21(1)	16(1)	21(1)	3(1)	-3(1)	-3(1)
N(8)	17(1)	21(1)	21(1)	1(1)	-6(1)	-1(1)
N(9)	32(1)	28(1)	20(1)	-3(1)	0(1)	-4(1)
N(10)	21(1)	24(1)	26(1)	4(1)	-10(1)	-5(1)
N(11)	18(1)	18(1)	18(1)	1(1)	-3(1)	-1(1)
N(12)	20(1)	21(1)	21(1)	3(1)	-2(1)	-7(1)
N(13)	22(1)	43(1)	28(1)	11(1)	-6(1)	-11(1)
N(14)	25(1)	35(1)	24(1)	7(1)	-3(1)	-7(1)
C(1)	14(1)	16(1)	17(1)	3(1)	-2(1)	-2(1)
C(2)	16(1)	18(1)	19(1)	4(1)	1(1)	-2(1)
C(3)	14(1)	19(1)	20(1)	3(1)	-1(1)	-3(1)
C(4)	15(1)	16(1)	16(1)	3(1)	-2(1)	-2(1)
C(5)	19(1)	20(1)	16(1)	4(1)	-2(1)	-4(1)
C(6)	17(1)	18(1)	17(1)	4(1)	0(1)	-3(1)
C(7)	21(1)	19(1)	21(1)	0(1)	2(1)	-6(1)
C(8)	22(1)	27(1)	24(1)	5(1)	-4(1)	-7(1)
C(9)	23(1)	27(1)	23(1)	4(1)	-1(1)	-7(1)
C(10)	21(1)	45(1)	30(1)	12(1)	-3(1)	-9(1)
O(31)	29(1)	46(1)	45(1)	19(1)	-12(1)	-10(1)
C(31)	72(2)	39(1)	68(2)	-7(1)	-8(1)	3(1)
C(32)	42(1)	31(1)	36(1)	4(1)	-15(1)	-12(1)
C(33)	75(2)	44(1)	40(1)	12(1)	-20(1)	-26(1)

Table S6. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for **10-(4-nitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4a**.

	x	y	z	U(eq)
H(1)	8349	9020	4881	19
H(2)	4668	9516	7209	22
H(3)	4620	7529	6381	22
H(4)	10584	7748	5470	19
H(5)	8629	7291	8186	23
H(6)	8497	5301	7378	22
H(7A)	6920	4151	6681	25
H(7B)	5529	5033	6150	25
H(8)	5837	3942	8661	29
H(10)	986	4866	8521	39
H(31A)	10649	638	8299	95
H(31B)	11683	1609	8703	95
H(31C)	11107	1997	7705	95
H(33A)	7419	2743	10153	75
H(33B)	9235	1987	10304	75
H(33C)	8203	1110	9817	75

Table S7. Torsion angles [°] for **10-(4-nitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4a**.

O(11)-N(14)-C(9)-C(8)	7.9(3)
O(11)-N(14)-C(9)-C(10)	-173.19(17)
O(12)-N(14)-C(9)-C(8)	-171.77(16)
O(12)-N(14)-C(9)-C(10)	7.2(3)
N(1)-C(1)-C(4)-N(5)	-2.09(15)
N(1)-C(1)-C(4)-N(6)	110.91(12)
N(1)-C(2)-C(3)-N(2)	1.82(13)
N(1)-C(2)-C(3)-N(4)	121.76(11)
N(2)-C(1)-C(4)-N(5)	-112.24(12)
N(2)-C(1)-C(4)-N(6)	0.76(14)
N(3)-C(2)-C(3)-N(2)	-118.03(11)
N(3)-C(2)-C(3)-N(4)	1.92(15)
N(3)-C(5)-C(6)-N(4)	-0.10(15)
N(3)-C(5)-C(6)-N(6)	119.95(11)
N(5)-C(5)-C(6)-N(4)	-117.75(12)
N(5)-C(5)-C(6)-N(6)	2.30(13)
N(7)-N(1)-C(1)-N(2)	-176.11(11)
N(7)-N(1)-C(1)-C(4)	67.42(15)
N(7)-N(1)-C(2)-N(3)	-53.20(16)
N(7)-N(1)-C(2)-C(3)	-168.98(11)
N(8)-N(2)-C(1)-N(1)	92.27(12)
N(8)-N(2)-C(1)-C(4)	-149.30(11)
N(8)-N(2)-C(3)-N(4)	133.77(12)
N(8)-N(2)-C(3)-C(2)	-107.35(12)

N(9)-N(3)-C(2)-N(1)	94.26(15)
N(9)-N(3)-C(2)-C(3)	-154.26(12)
N(9)-N(3)-C(5)-N(5)	-92.80(14)
N(9)-N(3)-C(5)-C(6)	153.27(12)
N(10)-N(5)-C(4)-N(6)	102.05(12)
N(10)-N(5)-C(4)-C(1)	-141.57(11)
N(10)-N(5)-C(5)-N(3)	128.64(13)
N(10)-N(5)-C(5)-C(6)	-115.34(13)
N(11)-N(6)-C(4)-N(5)	-96.63(12)
N(11)-N(6)-C(4)-C(1)	147.63(11)
N(11)-N(6)-C(6)-N(4)	-132.92(12)
N(11)-N(6)-C(6)-C(5)	108.48(12)
N(12)-N(13)-C(10)-C(9)	0.8(2)
N(12)-C(8)-C(9)-N(14)	178.54(15)
N(12)-C(8)-C(9)-C(10)	-0.60(18)
N(13)-N(12)-C(7)-N(4)	99.91(16)
N(13)-N(12)-C(8)-C(9)	1.14(18)
N(14)-C(9)-C(10)-N(13)	-179.24(16)
C(1)-N(1)-N(7)-O(1)	18.77(17)
C(1)-N(1)-N(7)-O(2)	-162.96(12)
C(1)-N(1)-C(2)-N(3)	89.09(14)
C(1)-N(1)-C(2)-C(3)	-26.70(14)
C(1)-N(2)-N(8)-O(3)	18.91(17)
C(1)-N(2)-N(8)-O(4)	-164.97(12)
C(1)-N(2)-C(3)-N(4)	-95.44(13)
C(1)-N(2)-C(3)-C(2)	23.44(13)
C(2)-N(1)-N(7)-O(1)	157.91(12)
C(2)-N(1)-N(7)-O(2)	-23.82(18)
C(2)-N(1)-C(1)-N(2)	41.15(13)
C(2)-N(1)-C(1)-C(4)	-75.32(13)
C(2)-N(3)-N(9)-O(5)	32.99(19)
C(2)-N(3)-N(9)-O(6)	-148.80(14)
C(2)-N(3)-C(5)-N(5)	57.41(16)
C(2)-N(3)-C(5)-C(6)	-56.52(15)
C(3)-N(2)-N(8)-O(3)	146.06(12)
C(3)-N(2)-N(8)-O(4)	-37.82(16)
C(3)-N(2)-C(1)-N(1)	-38.60(12)
C(3)-N(2)-C(1)-C(4)	79.83(12)
C(3)-N(4)-C(6)-N(6)	-58.33(15)
C(3)-N(4)-C(6)-C(5)	56.38(15)
C(3)-N(4)-C(7)-N(12)	-99.64(14)
C(4)-N(5)-N(10)-O(7)	35.93(17)
C(4)-N(5)-N(10)-O(8)	-148.75(13)
C(4)-N(5)-C(5)-N(3)	-96.98(13)
C(4)-N(5)-C(5)-C(6)	19.04(13)
C(4)-N(6)-N(11)-O(9)	-21.83(17)
C(4)-N(6)-N(11)-O(10)	163.26(12)
C(4)-N(6)-C(6)-N(4)	95.71(13)
C(4)-N(6)-C(6)-C(5)	-22.89(13)
C(5)-N(3)-N(9)-O(5)	-177.29(13)
C(5)-N(3)-N(9)-O(6)	0.9(2)

C(5)-N(3)-C(2)-N(1)	-55.82(16)
C(5)-N(3)-C(2)-C(3)	55.65(15)
C(5)-N(5)-N(10)-O(7)	166.80(12)
C(5)-N(5)-N(10)-O(8)	-17.88(19)
C(5)-N(5)-C(4)-N(6)	-33.69(13)
C(5)-N(5)-C(4)-C(1)	82.69(12)
C(6)-N(4)-C(3)-N(2)	57.91(16)
C(6)-N(4)-C(3)-C(2)	-57.45(15)
C(6)-N(4)-C(7)-N(12)	114.72(13)
C(6)-N(6)-N(11)-O(9)	-149.16(12)
C(6)-N(6)-N(11)-O(10)	35.94(17)
C(6)-N(6)-C(4)-N(5)	35.12(13)
C(6)-N(6)-C(4)-C(1)	-80.62(12)
C(7)-N(4)-C(3)-N(2)	-88.99(14)
C(7)-N(4)-C(3)-C(2)	155.66(11)
C(7)-N(4)-C(6)-N(6)	88.23(14)
C(7)-N(4)-C(6)-C(5)	-157.06(11)
C(7)-N(12)-N(13)-C(10)	-178.82(14)
C(7)-N(12)-C(8)-C(9)	178.53(14)
C(8)-N(12)-N(13)-C(10)	-1.22(19)
C(8)-N(12)-C(7)-N(4)	-77.32(18)
C(8)-C(9)-C(10)-N(13)	-0.1(2)

Symmetry transformations used to generate equivalent atoms:

Table S8. Crystal data and structure refinement for **10-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4d**.

Empirical formula	C14 H20 N16 O15
Formula weight	652.46
Temperature	100.00(10) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	P 2/c
Unit cell dimensions	a = 20.9929(2) Å α= 90°.
	b = 8.16100(10) Å α= 90.0440(10)°.
	c = 14.65210(10) Å γ= 90°.
Volume	2510.24(4) Å3
Z	4
Density (calculated)	1.726 g/cm3
Absorption coefficient	1.370 mm-1
F(000)	1344
Crystal size	0.07 x 0.04 x 0.02 mm3
Theta range for data collection	4.212 to 80.712°.
Index ranges	-26<=h<=26, -8<=k<=10, -18<=l<=18
Reflections collected	31539
Independent reflections	5444 [R(int) = 0.0330]
Observed reflections	5069
Completeness to theta = 67.684°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.81418
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	5444 / 4 / 432
Goodness-of-fit on F2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0997
R indices (all data)	R1 = 0.0397, wR2 = 0.1013
Extinction coefficient	0.00053(10)
Largest diff. peak and hole	0.404 and -0.276 e.Å-3

Table S9. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103) for **10-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4d**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	4982(1)	8608(1)	3493(1)	32(1)
O(2)	4110(1)	8879(1)	4277(1)	28(1)
O(3)	5880(1)	4041(1)	3636(1)	37(1)
O(4)	5744(1)	6364(1)	4339(1)	27(1)
O(5)	2492(1)	6498(1)	4574(1)	26(1)
O(6)	1546(1)	5898(1)	5067(1)	37(1)
O(7)	2415(1)	4269(1)	7477(1)	29(1)
O(8)	1440(1)	3982(2)	7002(1)	37(1)
O(9)	1396(1)	-787(2)	6403(1)	36(1)
O(10)	2326(1)	-1940(2)	6624(1)	34(1)

O(11)	3672(1)	1571(1)	7290(1)	26(1)
O(12)	3752(1)	-811(1)	6624(1)	27(1)
O(13)	2361(1)	-734(1)	2928(1)	28(1)
O(14)	1431(1)	-763(2)	3571(1)	33(1)
N(1)	4509(1)	8059(1)	3866(1)	22(1)
N(2)	5539(1)	5177(1)	3907(1)	22(1)
N(3)	4738(1)	2085(2)	3557(1)	29(1)
N(4)	3833(1)	5741(1)	3717(1)	21(1)
N(5)	3916(1)	4092(1)	3595(1)	19(1)
N(6)	3203(1)	2333(1)	4395(1)	17(1)
N(7)	2245(1)	3851(1)	4800(1)	18(1)
N(8)	2082(1)	5548(1)	4832(1)	23(1)
N(9)	2219(1)	2705(1)	6245(1)	19(1)
N(10)	2007(1)	3767(2)	6954(1)	24(1)
N(11)	2198(1)	-196(1)	5494(1)	20(1)
N(12)	1955(1)	-1018(2)	6228(1)	25(1)
N(13)	3163(1)	1137(1)	5983(1)	20(1)
N(14)	3549(1)	594(2)	6682(1)	21(1)
N(15)	2190(1)	949(1)	4114(1)	18(1)
N(16)	1976(1)	-308(2)	3505(1)	22(1)
C(1)	4412(1)	6306(2)	3805(1)	19(1)
C(2)	4883(1)	5082(2)	3725(1)	20(1)
C(3)	4538(1)	3629(2)	3614(1)	21(1)
C(4)	3359(1)	3038(2)	3507(1)	20(1)
C(5)	2923(1)	3495(2)	5022(1)	17(1)
C(6)	2899(1)	2766(2)	6013(1)	18(1)
C(7)	1859(1)	2786(2)	5388(1)	19(1)
C(8)	1834(1)	998(2)	4970(1)	19(1)
C(9)	2881(1)	784(2)	4368(1)	17(1)
C(10)	2878(1)	-11(2)	5348(1)	19(1)
O(15)	414(1)	2514(2)	4795(1)	38(1)
C(11)	773(2)	3408(8)	3348(3)	44(1)
C(12)	220(3)	2969(8)	3897(3)	51(1)
C(13)	-122(2)	2318(9)	5387(3)	55(1)
C(14)	88(2)	2069(10)	6332(3)	52(1)
C(15)	-91(10)	1880(40)	5330(15)	55(1)
C(16)	88(10)	1450(30)	6278(14)	52(1)
C(17)	279(12)	2560(40)	3852(11)	51(1)
C(18)	802(10)	2920(30)	3232(15)	44(1)

Table S10. Bond lengths [Å] and angles [°] for **10-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4d**.

O(1)-N(1)	1.2193(17)
O(2)-N(1)	1.2293(16)
O(3)-N(2)	1.2364(16)
O(4)-N(2)	1.2345(16)
O(5)-N(8)	1.2198(17)
O(6)-N(8)	1.2113(17)
O(7)-N(10)	1.2194(17)
O(8)-N(10)	1.2049(17)

O(9)-N(12)	1.2167(18)
O(10)-N(12)	1.2278(17)
O(11)-N(14)	1.2222(16)
O(12)-N(14)	1.2263(16)
O(13)-N(16)	1.2205(17)
O(14)-N(16)	1.2066(17)
N(1)-C(1)	1.4479(17)
N(2)-C(2)	1.4056(18)
N(3)-H(3A)	0.92(2)
N(3)-H(3B)	0.91(2)
N(3)-C(3)	1.3307(19)
N(4)-N(5)	1.3684(16)
N(4)-C(1)	1.3062(18)
N(5)-C(3)	1.3596(18)
N(5)-C(4)	1.4581(17)
N(6)-C(4)	1.4595(17)
N(6)-C(5)	1.4456(16)
N(6)-C(9)	1.4342(16)
N(7)-N(8)	1.4272(16)
N(7)-C(5)	1.4885(16)
N(7)-C(7)	1.4685(17)
N(9)-N(10)	1.4244(16)
N(9)-C(6)	1.4696(17)
N(9)-C(7)	1.4661(16)
N(11)-N(12)	1.3672(16)
N(11)-C(8)	1.4575(17)
N(11)-C(10)	1.4502(17)
N(13)-N(14)	1.3784(15)
N(13)-C(6)	1.4411(16)
N(13)-C(10)	1.4501(17)
N(15)-N(16)	1.4323(15)
N(15)-C(8)	1.4605(17)
N(15)-C(9)	1.5029(16)
C(1)-C(2)	1.4094(18)
C(2)-C(3)	1.3982(19)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-H(5)	1.0000
C(5)-C(6)	1.5690(17)
C(6)-H(6)	1.0000
C(7)-H(7)	1.0000
C(7)-C(8)	1.5833(18)
C(8)-H(8)	1.0000
C(9)-H(9)	1.0000
C(9)-C(10)	1.5752(18)
C(10)-H(10)	1.0000
O(15)-C(12)	1.427(4)
O(15)-C(13)	1.431(4)
O(15)-C(15)	1.415(16)
O(15)-C(17)	1.411(16)
C(11)-H(11A)	0.9800

C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(11)-C(12)	1.458(5)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(13)-C(14)	1.467(5)
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(15)-C(16)	1.482(17)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(17)-C(18)	1.456(17)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800

O(1)-N(1)-O(2)	125.08(12)
O(1)-N(1)-C(1)	116.69(12)
O(2)-N(1)-C(1)	118.23(12)
O(3)-N(2)-C(2)	117.71(12)
O(4)-N(2)-O(3)	123.46(12)
O(4)-N(2)-C(2)	118.82(11)
H(3A)-N(3)-H(3B)	117(2)
C(3)-N(3)-H(3A)	120.1(14)
C(3)-N(3)-H(3B)	120.3(15)
C(1)-N(4)-N(5)	103.96(11)
N(4)-N(5)-C(4)	119.32(11)
C(3)-N(5)-N(4)	113.15(11)
C(3)-N(5)-C(4)	127.46(11)
C(5)-N(6)-C(4)	113.57(10)
C(9)-N(6)-C(4)	115.38(10)
C(9)-N(6)-C(5)	113.80(10)
N(8)-N(7)-C(5)	114.33(10)
N(8)-N(7)-C(7)	114.97(11)
C(7)-N(7)-C(5)	106.45(10)
O(5)-N(8)-N(7)	115.90(11)
O(6)-N(8)-O(5)	126.48(12)
O(6)-N(8)-N(7)	117.52(12)
N(10)-N(9)-C(6)	116.88(10)
N(10)-N(9)-C(7)	115.90(10)
C(7)-N(9)-C(6)	107.44(10)
O(7)-N(10)-N(9)	116.31(12)
O(8)-N(10)-O(7)	127.45(13)

O(8)-N(10)-N(9)	116.06(12)
N(12)-N(11)-C(8)	123.14(11)
N(12)-N(11)-C(10)	122.37(11)
C(10)-N(11)-C(8)	111.62(10)
O(9)-N(12)-O(10)	127.41(13)
O(9)-N(12)-N(11)	116.77(12)
O(10)-N(12)-N(11)	115.79(12)
N(14)-N(13)-C(6)	119.98(11)
N(14)-N(13)-C(10)	120.79(11)
C(6)-N(13)-C(10)	117.17(10)
O(11)-N(14)-O(12)	125.95(12)
O(11)-N(14)-N(13)	117.12(11)
O(12)-N(14)-N(13)	116.90(11)
N(16)-N(15)-C(8)	113.21(10)
N(16)-N(15)-C(9)	113.10(10)
C(8)-N(15)-C(9)	106.53(10)
O(13)-N(16)-N(15)	115.38(11)
O(14)-N(16)-O(13)	126.62(12)
O(14)-N(16)-N(15)	117.82(11)
N(4)-C(1)-N(1)	119.01(12)
N(4)-C(1)-C(2)	113.18(12)
C(2)-C(1)-N(1)	127.41(12)
N(2)-C(2)-C(1)	129.19(12)
C(3)-C(2)-N(2)	125.15(12)
C(3)-C(2)-C(1)	104.39(12)
N(3)-C(3)-N(5)	124.38(13)
N(3)-C(3)-C(2)	130.36(14)
N(5)-C(3)-C(2)	105.25(12)
N(5)-C(4)-N(6)	109.54(10)
N(5)-C(4)-H(4A)	109.8
N(5)-C(4)-H(4B)	109.8
N(6)-C(4)-H(4A)	109.8
N(6)-C(4)-H(4B)	109.8
H(4A)-C(4)-H(4B)	108.2
N(6)-C(5)-N(7)	112.21(10)
N(6)-C(5)-H(5)	109.9
N(6)-C(5)-C(6)	110.63(10)
N(7)-C(5)-H(5)	109.9
N(7)-C(5)-C(6)	104.23(10)
C(6)-C(5)-H(5)	109.9
N(9)-C(6)-C(5)	105.00(10)
N(9)-C(6)-H(6)	111.1
N(13)-C(6)-N(9)	110.45(11)
N(13)-C(6)-C(5)	108.04(10)
N(13)-C(6)-H(6)	111.1
C(5)-C(6)-H(6)	111.1
N(7)-C(7)-H(7)	111.6
N(7)-C(7)-C(8)	109.67(10)
N(9)-C(7)-N(7)	104.23(10)
N(9)-C(7)-H(7)	111.6
N(9)-C(7)-C(8)	107.90(10)

C(8)-C(7)-H(7)	111.6
N(11)-C(8)-N(15)	99.51(10)
N(11)-C(8)-C(7)	113.22(10)
N(11)-C(8)-H(8)	111.2
N(15)-C(8)-C(7)	109.91(10)
N(15)-C(8)-H(8)	111.2
C(7)-C(8)-H(8)	111.2
N(6)-C(9)-N(15)	112.51(10)
N(6)-C(9)-H(9)	109.8
N(6)-C(9)-C(10)	109.91(10)
N(15)-C(9)-H(9)	109.8
N(15)-C(9)-C(10)	104.93(10)
C(10)-C(9)-H(9)	109.8
N(11)-C(10)-C(9)	100.52(10)
N(11)-C(10)-H(10)	111.7
N(13)-C(10)-N(11)	112.21(11)
N(13)-C(10)-C(9)	108.46(10)
N(13)-C(10)-H(10)	111.7
C(9)-C(10)-H(10)	111.7
C(12)-O(15)-C(13)	111.3(3)
C(17)-O(15)-C(15)	113.6(15)
H(11A)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(12)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11C)	109.5
O(15)-C(12)-C(11)	110.2(4)
O(15)-C(12)-H(12A)	109.6
O(15)-C(12)-H(12B)	109.6
C(11)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
O(15)-C(13)-H(13A)	109.5
O(15)-C(13)-H(13B)	109.5
O(15)-C(13)-C(14)	110.5(4)
H(13A)-C(13)-H(13B)	108.1
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
O(15)-C(15)-H(15A)	108.6
O(15)-C(15)-H(15B)	108.6
O(15)-C(15)-C(16)	114.6(18)
H(15A)-C(15)-H(15B)	107.6
C(16)-C(15)-H(15A)	108.6
C(16)-C(15)-H(15B)	108.6

C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(15)-C(17)-H(17A)	107.9
O(15)-C(17)-H(17B)	107.9
O(15)-C(17)-C(18)	117.7(19)
H(17A)-C(17)-H(17B)	107.2
C(18)-C(17)-H(17A)	107.9
C(18)-C(17)-H(17B)	107.9
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Table S11. Anisotropic displacement parameters (Å2x 103) for **10-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4d**. The anisotropic displacement factor exponent takes the form: -2p2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	26(1)	21(1)	51(1)	5(1)	6(1)	-4(1)
O(2)	26(1)	20(1)	36(1)	-4(1)	0(1)	4(1)
O(3)	24(1)	25(1)	62(1)	-6(1)	1(1)	6(1)
O(4)	24(1)	28(1)	29(1)	-2(1)	-4(1)	-3(1)
O(5)	32(1)	16(1)	31(1)	2(1)	0(1)	1(1)
O(6)	26(1)	26(1)	60(1)	0(1)	3(1)	8(1)
O(7)	35(1)	27(1)	25(1)	-8(1)	-5(1)	0(1)
O(8)	28(1)	50(1)	35(1)	-15(1)	2(1)	8(1)
O(9)	27(1)	46(1)	33(1)	9(1)	8(1)	-1(1)
O(10)	36(1)	33(1)	32(1)	14(1)	0(1)	3(1)
O(11)	28(1)	32(1)	21(1)	-3(1)	-7(1)	3(1)
O(12)	27(1)	20(1)	32(1)	5(1)	-5(1)	5(1)
O(13)	31(1)	31(1)	24(1)	-10(1)	-1(1)	-1(1)
O(14)	28(1)	40(1)	32(1)	-9(1)	-3(1)	-13(1)
N(1)	21(1)	16(1)	29(1)	1(1)	-3(1)	0(1)
N(2)	22(1)	19(1)	25(1)	2(1)	-1(1)	0(1)
N(3)	27(1)	16(1)	44(1)	-1(1)	2(1)	1(1)
N(4)	22(1)	16(1)	23(1)	2(1)	-1(1)	0(1)
N(5)	21(1)	15(1)	22(1)	1(1)	-1(1)	-2(1)
N(6)	20(1)	14(1)	18(1)	-1(1)	-1(1)	-1(1)
N(7)	20(1)	15(1)	21(1)	0(1)	-3(1)	2(1)
N(8)	25(1)	18(1)	26(1)	-1(1)	-5(1)	4(1)
N(9)	21(1)	20(1)	17(1)	-3(1)	-2(1)	2(1)
N(10)	29(1)	23(1)	20(1)	-4(1)	-1(1)	2(1)

N(11)	21(1)	18(1)	21(1)	3(1)	0(1)	-1(1)
N(12)	28(1)	25(1)	22(1)	3(1)	2(1)	-4(1)
N(13)	22(1)	17(1)	20(1)	0(1)	-6(1)	2(1)
N(14)	19(1)	24(1)	20(1)	4(1)	-3(1)	1(1)
N(15)	19(1)	17(1)	19(1)	-2(1)	-2(1)	-2(1)
N(16)	25(1)	21(1)	21(1)	-3(1)	-4(1)	-3(1)
C(1)	22(1)	16(1)	20(1)	2(1)	-1(1)	-1(1)
C(2)	21(1)	16(1)	22(1)	2(1)	0(1)	0(1)
C(3)	23(1)	20(1)	20(1)	1(1)	0(1)	-1(1)
C(4)	21(1)	20(1)	19(1)	1(1)	-2(1)	-4(1)
C(5)	18(1)	15(1)	18(1)	-1(1)	-3(1)	1(1)
C(6)	20(1)	16(1)	19(1)	-1(1)	-3(1)	1(1)
C(7)	20(1)	19(1)	19(1)	-1(1)	-2(1)	1(1)
C(8)	19(1)	18(1)	20(1)	-1(1)	-2(1)	-1(1)
C(9)	18(1)	15(1)	19(1)	-1(1)	-2(1)	-1(1)
C(10)	21(1)	15(1)	20(1)	0(1)	-2(1)	-1(1)
O(15)	26(1)	49(1)	40(1)	4(1)	-6(1)	-1(1)
C(11)	44(1)	48(3)	37(2)	8(2)	-12(1)	-1(2)
C(12)	40(2)	65(3)	49(1)	13(2)	-16(1)	3(2)
C(13)	26(1)	84(4)	54(1)	-4(2)	2(1)	0(2)
C(14)	32(1)	75(3)	48(1)	0(2)	4(1)	-11(2)
C(15)	26(1)	84(4)	54(1)	-4(2)	2(1)	0(2)
C(16)	32(1)	75(3)	48(1)	0(2)	4(1)	-11(2)
C(17)	40(2)	65(3)	49(1)	13(2)	-16(1)	3(2)
C(18)	44(1)	48(3)	37(2)	8(2)	-12(1)	-1(2)

Table S12. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for **10-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4d**.

	x	y	z	U(eq)
H(3A)	5165(11)	1860(30)	3522(14)	36(5)
H(3B)	4475(11)	1250(30)	3712(16)	43(6)
H(4A)	3448	2150	3065	24
H(4B)	2993	3683	3278	24
H(5)	3175	4535	5021	21
H(6)	3139	3474	6451	22
H(7)	1423	3243	5484	23
H(8)	1384	627	4880	23
H(9)	3100	37	3928	21
H(10)	3102	-1092	5354	23
H(11A)	644	3535	2709	65
H(11B)	1095	2543	3395	65
H(11C)	952	4443	3571	65
H(12A)	-76	3911	3930	62
H(12B)	-8	2043	3607	62
H(13A)	-378	1365	5186	66
H(13B)	-395	3305	5353	66
H(14A)	392	1156	6355	77
H(14B)	-281	1815	6716	77

H(14C)	295	3068	6556	77
H(15A)	-262	895	5025	66
H(15B)	-436	2708	5350	66
H(16A)	109	252	6337	77
H(16B)	-232	1880	6701	77
H(16C)	505	1921	6422	77
H(17A)	-58	3388	3751	62
H(17B)	99	1481	3678	62
H(18A)	653	3655	2749	65
H(18B)	957	1896	2959	65
H(18C)	1149	3444	3571	65

Table S13. Torsion angles [°] for **10-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4d**.

O(1)-N(1)-C(1)-N(4)	-143.23(13)
O(1)-N(1)-C(1)-C(2)	29.0(2)
O(2)-N(1)-C(1)-N(4)	36.06(18)
O(2)-N(1)-C(1)-C(2)	-151.73(14)
O(3)-N(2)-C(2)-C(1)	-167.38(14)
O(3)-N(2)-C(2)-C(3)	27.6(2)
O(4)-N(2)-C(2)-C(1)	13.9(2)
O(4)-N(2)-C(2)-C(3)	-151.21(14)
N(1)-C(1)-C(2)-N(2)	17.4(2)
N(1)-C(1)-C(2)-C(3)	-175.14(13)
N(2)-C(2)-C(3)-N(3)	-7.7(2)
N(2)-C(2)-C(3)-N(5)	170.72(12)
N(4)-N(5)-C(3)-N(3)	176.49(13)
N(4)-N(5)-C(3)-C(2)	-2.07(15)
N(4)-N(5)-C(4)-N(6)	-95.48(13)
N(4)-C(1)-C(2)-N(2)	-169.99(13)
N(4)-C(1)-C(2)-C(3)	-2.56(16)
N(5)-N(4)-C(1)-N(1)	174.58(12)
N(5)-N(4)-C(1)-C(2)	1.31(15)
N(6)-C(5)-C(6)-N(9)	-118.39(11)
N(6)-C(5)-C(6)-N(13)	-0.51(14)
N(6)-C(9)-C(10)-N(11)	121.94(11)
N(6)-C(9)-C(10)-N(13)	4.08(14)
N(7)-C(5)-C(6)-N(9)	2.42(12)
N(7)-C(5)-C(6)-N(13)	120.30(11)
N(7)-C(7)-C(8)-N(11)	109.10(12)
N(7)-C(7)-C(8)-N(15)	-1.17(14)
N(8)-N(7)-C(5)-N(6)	-135.28(11)
N(8)-N(7)-C(5)-C(6)	104.97(12)
N(8)-N(7)-C(7)-N(9)	-92.29(12)
N(8)-N(7)-C(7)-C(8)	152.41(10)
N(9)-C(7)-C(8)-N(11)	-3.84(15)
N(9)-C(7)-C(8)-N(15)	-114.12(11)
N(10)-N(9)-C(6)-N(13)	130.75(11)
N(10)-N(9)-C(6)-C(5)	-113.01(12)
N(10)-N(9)-C(7)-N(7)	98.77(12)

N(10)-N(9)-C(7)-C(8)	-144.69(11)
N(12)-N(11)-C(8)-N(15)	-157.55(12)
N(12)-N(11)-C(8)-C(7)	85.86(15)
N(12)-N(11)-C(10)-N(13)	-72.43(15)
N(12)-N(11)-C(10)-C(9)	172.51(11)
N(14)-N(13)-C(6)-N(9)	-105.20(13)
N(14)-N(13)-C(6)-C(5)	140.48(12)
N(14)-N(13)-C(10)-N(11)	107.60(13)
N(14)-N(13)-C(10)-C(9)	-142.28(12)
N(15)-C(9)-C(10)-N(11)	0.74(12)
N(15)-C(9)-C(10)-N(13)	-117.12(11)
N(16)-N(15)-C(8)-N(11)	86.76(12)
N(16)-N(15)-C(8)-C(7)	-154.17(10)
N(16)-N(15)-C(9)-N(6)	139.50(11)
N(16)-N(15)-C(9)-C(10)	-101.03(11)
C(1)-N(4)-N(5)-C(3)	0.51(15)
C(1)-N(4)-N(5)-C(4)	177.58(11)
C(1)-C(2)-C(3)-N(3)	-175.82(15)
C(1)-C(2)-C(3)-N(5)	2.62(14)
C(3)-N(5)-C(4)-N(6)	81.13(16)
C(4)-N(5)-C(3)-N(3)	-0.3(2)
C(4)-N(5)-C(3)-C(2)	-178.85(12)
C(4)-N(6)-C(5)-N(7)	75.77(13)
C(4)-N(6)-C(5)-C(6)	-168.29(10)
C(4)-N(6)-C(9)-N(15)	-75.92(14)
C(4)-N(6)-C(9)-C(10)	167.55(10)
C(5)-N(6)-C(4)-N(5)	73.18(13)
C(5)-N(6)-C(9)-N(15)	57.94(14)
C(5)-N(6)-C(9)-C(10)	-58.59(13)
C(5)-N(7)-N(8)-O(5)	35.93(16)
C(5)-N(7)-N(8)-O(6)	-147.52(13)
C(5)-N(7)-C(7)-N(9)	35.41(12)
C(5)-N(7)-C(7)-C(8)	-79.89(12)
C(6)-N(9)-N(10)-O(7)	-20.59(17)
C(6)-N(9)-N(10)-O(8)	163.95(12)
C(6)-N(9)-C(7)-N(7)	-34.02(13)
C(6)-N(9)-C(7)-C(8)	82.52(12)
C(6)-N(13)-N(14)-O(11)	-3.01(18)
C(6)-N(13)-N(14)-O(12)	178.99(12)
C(6)-N(13)-C(10)-N(11)	-56.10(15)
C(6)-N(13)-C(10)-C(9)	54.03(15)
C(7)-N(7)-N(8)-O(5)	159.54(11)
C(7)-N(7)-N(8)-O(6)	-23.91(17)
C(7)-N(7)-C(5)-N(6)	96.64(12)
C(7)-N(7)-C(5)-C(6)	-23.11(12)
C(7)-N(9)-N(10)-O(7)	-148.87(12)
C(7)-N(9)-N(10)-O(8)	35.66(17)
C(7)-N(9)-C(6)-N(13)	-96.99(12)
C(7)-N(9)-C(6)-C(5)	19.24(13)
C(8)-N(11)-N(12)-O(9)	4.37(19)
C(8)-N(11)-N(12)-O(10)	-177.31(12)

C(8)-N(11)-C(10)-N(13)	88.93(13)
C(8)-N(11)-C(10)-C(9)	-26.14(13)
C(8)-N(15)-N(16)-O(13)	-158.60(12)
C(8)-N(15)-N(16)-O(14)	25.95(17)
C(8)-N(15)-C(9)-N(6)	-95.50(12)
C(8)-N(15)-C(9)-C(10)	23.97(12)
C(9)-N(6)-C(4)-N(5)	-152.86(11)
C(9)-N(6)-C(5)-N(7)	-58.93(14)
C(9)-N(6)-C(5)-C(6)	57.01(14)
C(9)-N(15)-N(16)-O(13)	-37.30(15)
C(9)-N(15)-N(16)-O(14)	147.26(12)
C(9)-N(15)-C(8)-N(11)	-38.17(12)
C(9)-N(15)-C(8)-C(7)	80.90(12)
C(10)-N(11)-N(12)-O(9)	163.58(13)
C(10)-N(11)-N(12)-O(10)	-18.10(19)
C(10)-N(11)-C(8)-N(15)	41.26(13)
C(10)-N(11)-C(8)-C(7)	-75.33(13)
C(10)-N(13)-N(14)-O(11)	-166.24(12)
C(10)-N(13)-N(14)-O(12)	15.75(18)
C(10)-N(13)-C(6)-N(9)	58.63(15)
C(10)-N(13)-C(6)-C(5)	-55.69(14)
C(12)-O(15)-C(13)-C(14)	-172.5(4)
C(13)-O(15)-C(12)-C(11)	171.2(4)
C(15)-O(15)-C(17)-C(18)	-170(2)
C(17)-O(15)-C(15)-C(16)	166(2)

Table S14. Hydrogen bonds for **1010-(5-amino-3,4-dinitropyrazol-1-yl)methyl-2,4,6,8,12-pentanitro-2,4,6,8,10,12-hexaazaisowurtzitane 4d** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3A)...O(3)	0.92(2)	2.33(2)	2.8825(18)	118.1(17)
N(3)-H(3A)...O(12)#1	0.92(2)	2.44(2)	3.3478(17)	170.8(19)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1

X-ray crystallographic data and refinement details.

X-ray diffraction data were collected at 100K on a four-circle Rigaku Synergy S diffractometer equipped with a HyPix600HE area-detector (kappa geometry, shutterless ω-scan technique), using monochromatized Cu K_α-radiation. The intensity data were integrated and corrected for absorption and decay by the CrysAlisPro program[S1]. The structure was solved by direct methods using SHELXT[S2] and refined on F^2 using SHELXL-2018[S3] in the OLEX2 program. All non-hydrogen atoms were refined with individual anisotropic displacement parameters. Locations of amino hydrogen atoms (H3A, H3B) were found from the electron density-difference map; these hydrogen atoms were refined with individual isotropic displacement parameters. All other hydrogen atoms were placed in ideal calculated positions and refined as riding atoms with relative isotropic displacement parameters.

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Refinement details determination of physico-chemical and detonation properties.

The sensitivity to impact and friction was determined according to the standards[S4,S5], details are given in [S5]. The thermal behavior of 0.1-0.5 mg samples was determined using a Netzsch STA 449 F1 device when heated at a rate of 5 K/min. The enthalpy of formation in the gas phase was calculated using the semi-empirical AIQM1 method[S6] implemented in the MLatom software package[S7]. The method is based on the semi-empirical ODM2 method[S8], uses the D4 variance correction[S9] and the ANI-1x neuro-network potential correction[S10]. For the transition to the solid phase, the enthalpy of sublimation was calculated using the modified Trouton equation[S11]. It should be noted that although the difference in the calculated value of the enthalpy of CL-20 formation from the known experimental value[S12] exceeds the experimental error, this does not significantly contribute to the values of the detonation parameters. The detonation parameters were calculated using empirical equations implemented in the PILEM application[S13], experimental parameter values for CL-20 are also taken from[S14].

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