Supporting Information for

Impact of regiochemistry in energetic materials science: a case of (nitratomethyl-1,2,3-triazolyl)furazans

Margarita A. Epishina,[1] Alexander S. Kulikov,[1] Ivan V. Ananyev,[2,3] Aleksei A. Anisimov,[3,4] Konstantin A. Monogarov,[5] Leonid L. Fershtat*[1]

[1.] N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Leninsky Prosp. 47, Moscow 119991 (Russian Federation).

[2.] N.S. Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, GSP-1, Leninsky prospect, 31, 119991 Moscow, Russia.

[3.] National Research University Higher School of Economics 101000, Myasnitskaya str., 20, Moscow (Russian Federation).

[4.] Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilova st, Moscow, Russia, 119991

[5.] N. N. Semenov Federal Research Centre for Chemical Physics, Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991 (Russian Federation).

*E-mail: fershtat@bk.ru

Table of Contents

S1. Crystallographic data

Table S1. Crystallographic details and refinement parameters for **3c** and **4a**.

	3c	**4a**
Formula	$C_6H_6N_6O_5$	$C_5H_3N_7O_6$
Mass	242.17	257.14
T, K	100	100
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	$P2_1/n$
Z (Z')	8 (1)	4 (1)
a, Å	18.5628(3)	11.2782(3)
b, Å	7.92780(10)	6.3430(2)
c, Å	13.6589(2)	13.7366(4)
α, °	90	90
β, °	111.2210(10)	104.6130(10)
γ, °	90	90
V, $Å^3$	1873.77(5)	950.90(5)
d_{cryst}, $g \cdot cm^{-3}$	1.717	1.796
F(000)	992	520
$2\theta_{max}$, °	60	58
Number of reflections measured	25668	11887
Independent reflections	2710	2533
Reflections with I>2σ(I)	2598	2374
Number of parameters	178	175
R_1	0.0299	0.0306
wR_2	0.0777	0.0840
GOF	1.040	1.038
Residual electron density, $e \cdot Å^{-3}$ (d_{min}/d_{max})	0.481/-0.213	0.392/-0.277

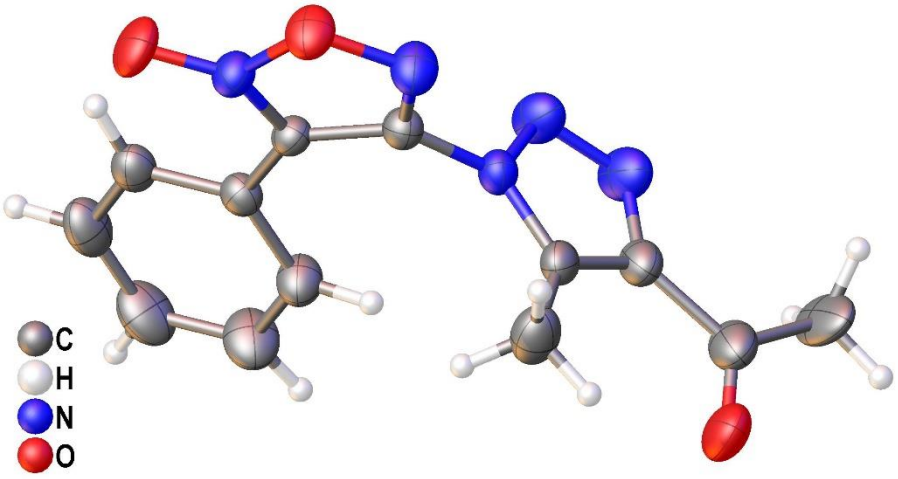


Figure S1. A general view of the independent unit of the FAZGOF structure.

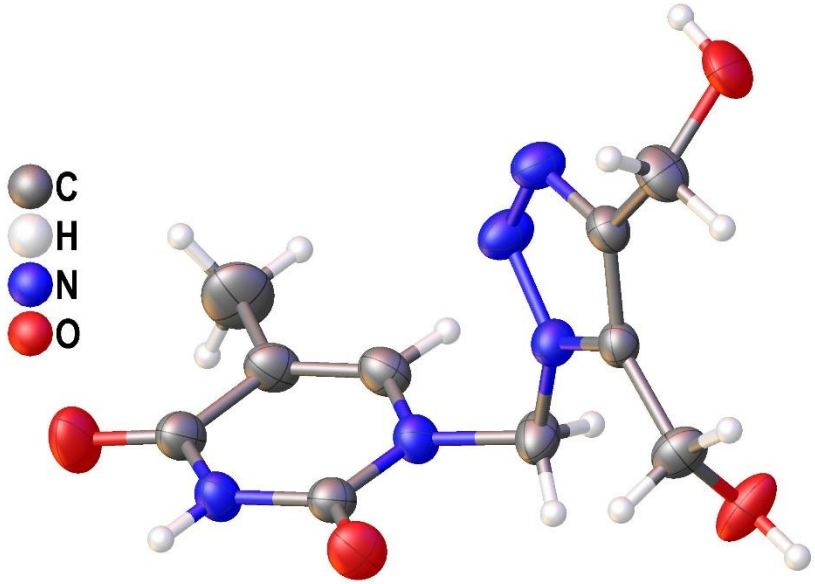


Figure S2. A general view of the independent unit of the YASJIM structure.

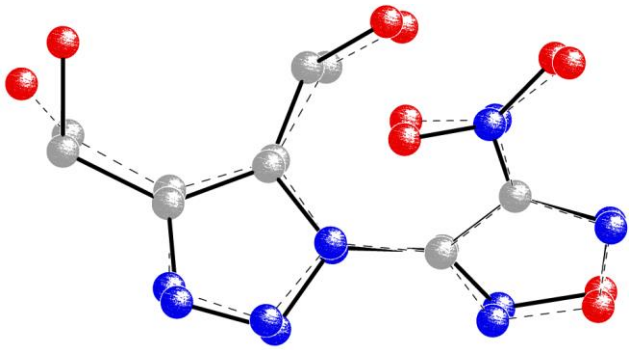


Figure S3. The best root-mean-square overlap for the non-hydrogen atoms of the crystal (dashed lines) and the equilibrium isolated (full lines) molecular conformations of **3c**.

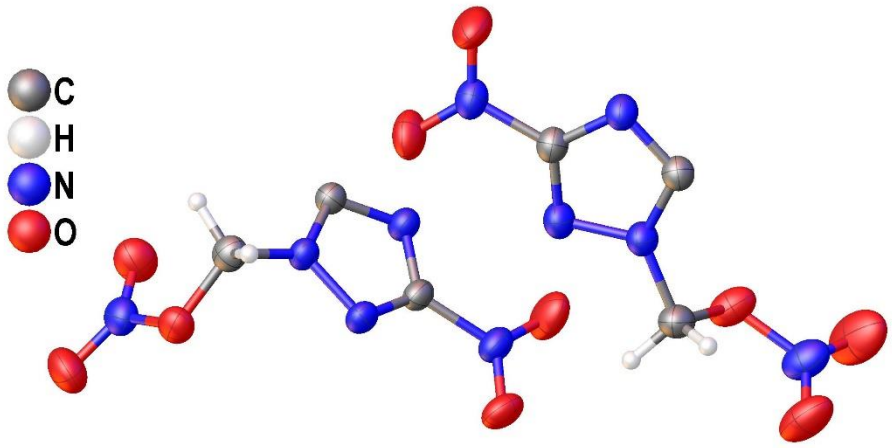


Figure S4. A general view of the independent unit of the ELIGUD structure.

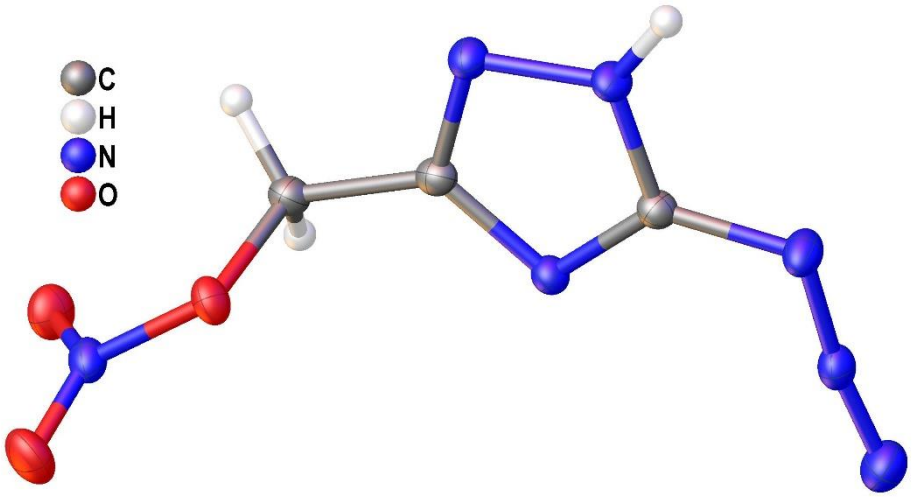


Figure S5. A general view of the independent unit of the ZUJCUF structure.

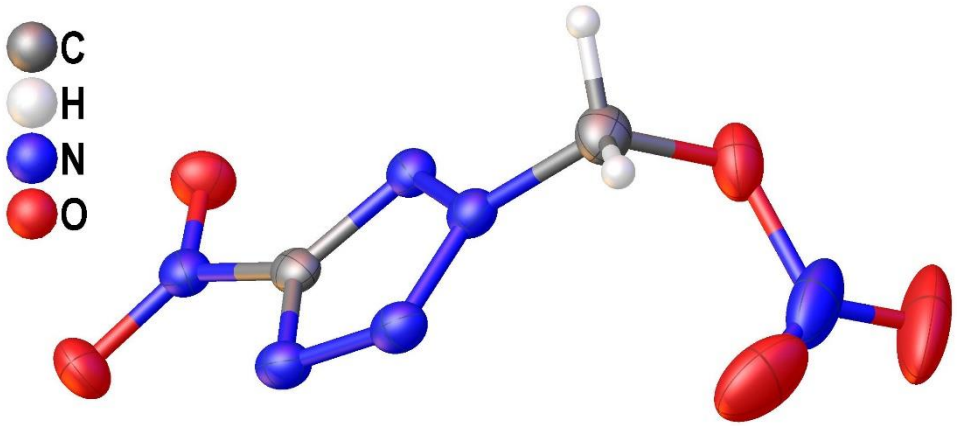


Figure S6. A general view of the independent unit of the HEGLEM structure.

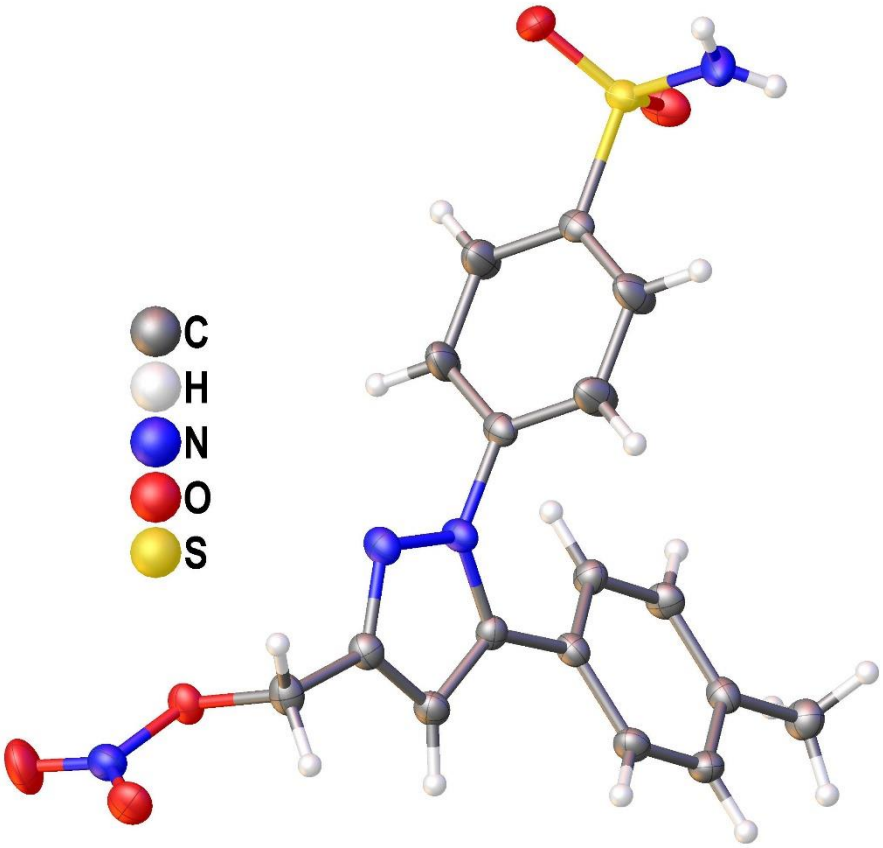


Figure S7. A general view of the independent unit of the KOXWIF structure.

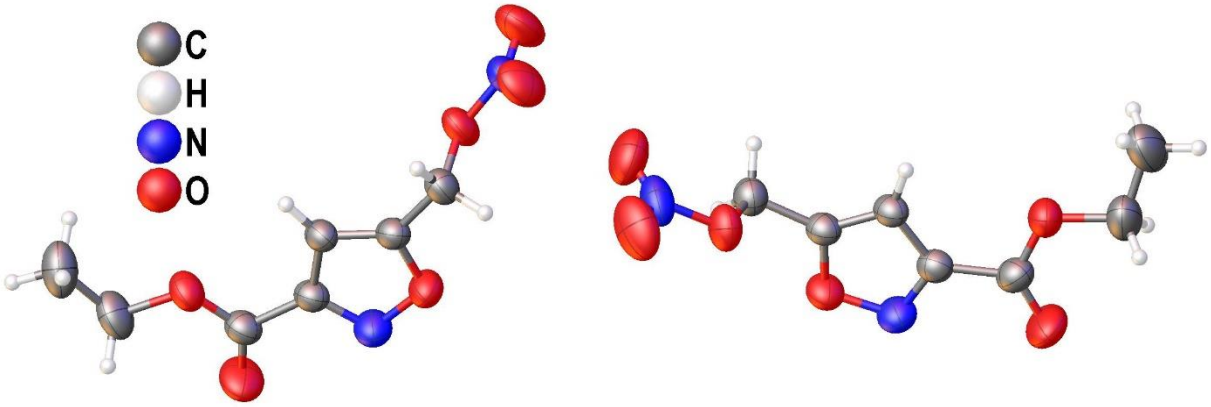


Figure S8. A general view of the independent unit of the NILZAM structure.

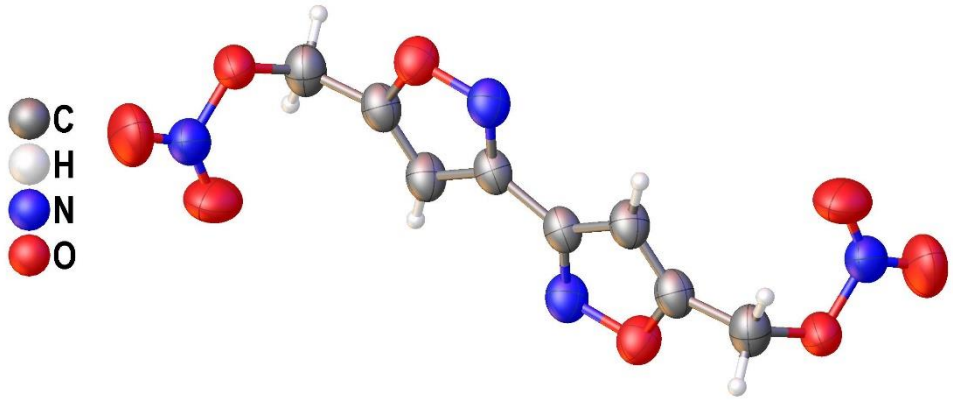


Figure S9. A general view of the molecule in the TAXDUU structure.

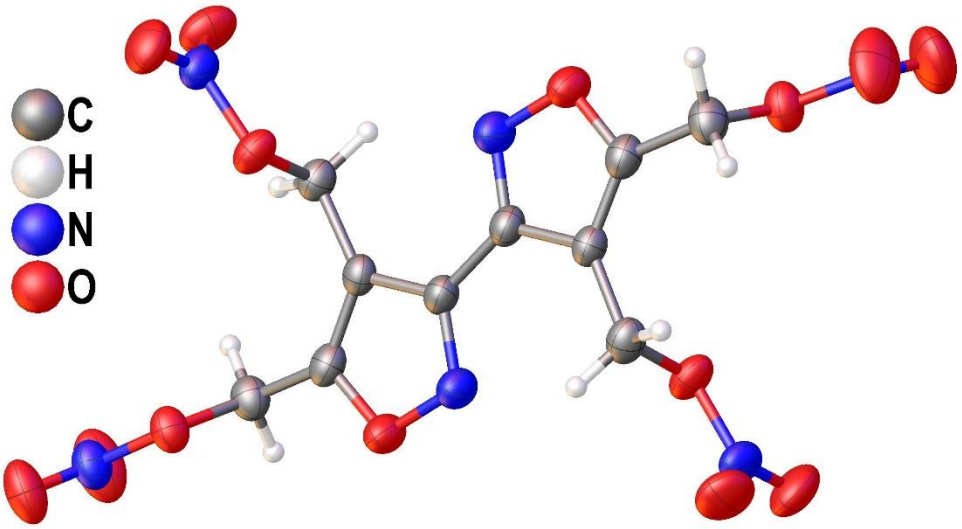


Figure S10. A general view of the independent unit of the WANVEP structure.

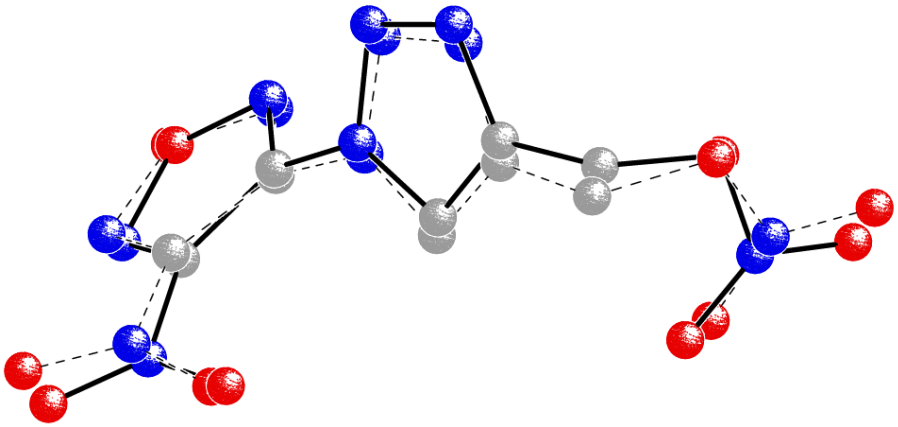


Figure S11. The best root-mean-square overlap for the non-hydrogen atoms of the crystal (dashed lines) and the equilibrium isolated (full lines) molecular conformations of **4a**.

S2. Computational details

A general formula used for the calculation of the enthalpies of formation was as follows:

$$\Delta_f H^0_{(g)} = \Sigma H_{atom} - \Sigma \Delta_{thermal} H_{atom} - \Sigma D_0$$

$$\Sigma D_0 = \Sigma CBS\text{-}4M(H_{atom}) - CBS\text{-}4M(H_{molecule})$$

Corrections on values of enthalpies of sublimation and enthalpies of vaporization were calculated according to empirical formulae:

$$\Delta_f H^0_{(subl)} = 0.04476 \cdot T_m$$

$$\Delta_f H^0_{(vap)} = 0.02095 \cdot T_{vap}$$

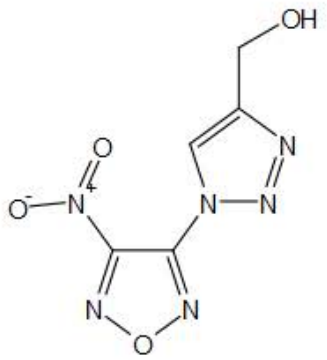
Table S2. Atomic contributions to the enthalpies of formation.

	multiplicity	$\Delta_f H^0$ (0K), kcal mol^{-1}	Thermal ΔΔH, kcal mol^{-1}	CBS-4M, hartree
H	2	51.63	1.01	-0.500991
C	3	169.98	0.25	-37.786156
N	4	112.53	1.04	-54.522462
O	3	58.99	1.04	-74.991202

Table S3. Calculated enthalpies of formation.

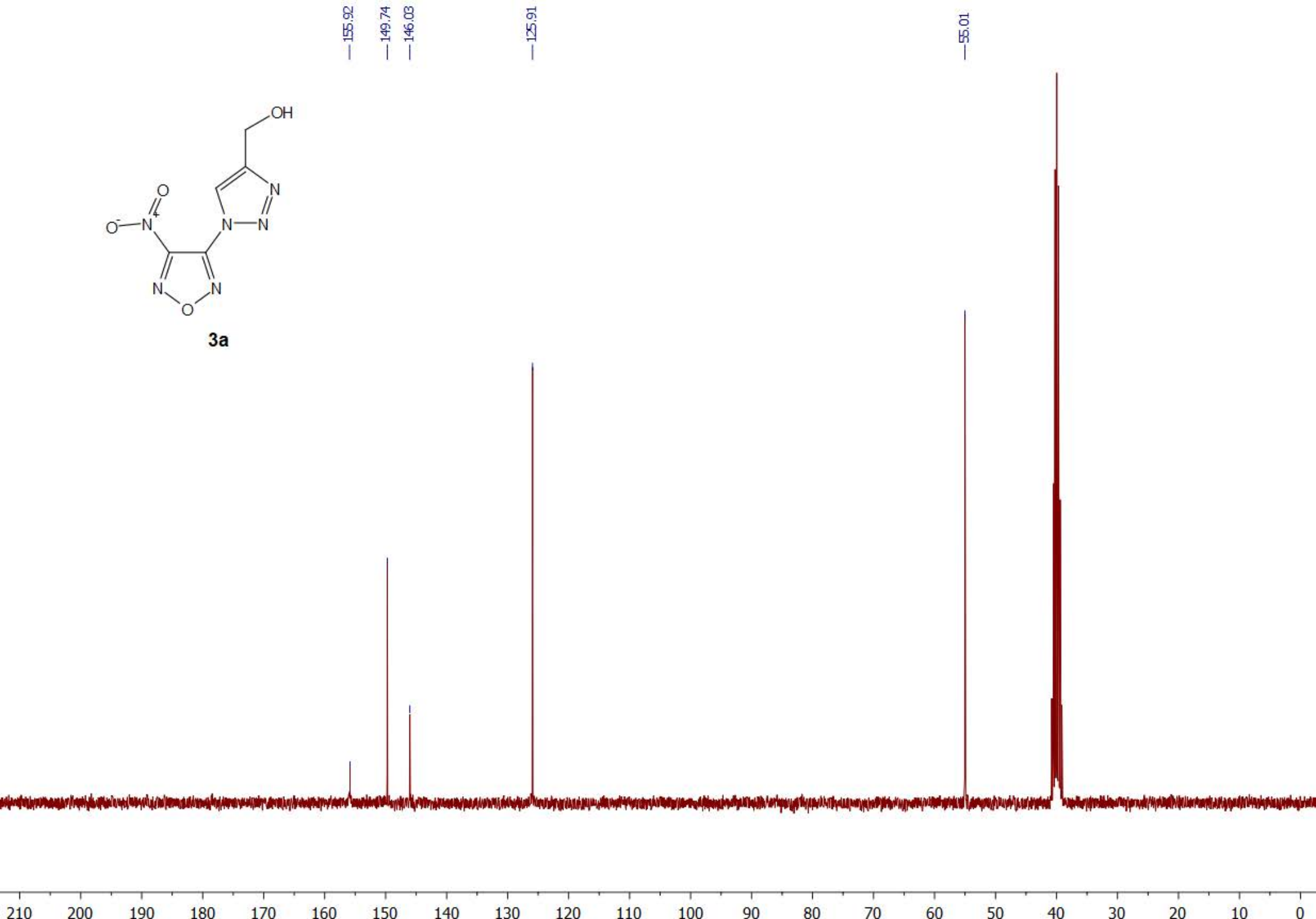
	4a	**4b**	**4c**
CBS-4($H_{molecule}$), hartree	-1025.297561	-1025.294723	-1343.93672
ΣCBS-4M(H_{atom}), hartree	-1022.038199	-1022.038199	-1339.821414
ΣD_0, hartree	3.259362	3.256524	4.115306
$\Delta_f H^0_{(g)}$, kcal mol^{-1}	83.4	85.2	52.0
$\Delta_f H^0_{(cond)}$, kcal mol^{-1}	67.9 (solid)	76.0 (liquid)	42.9 (liquid)

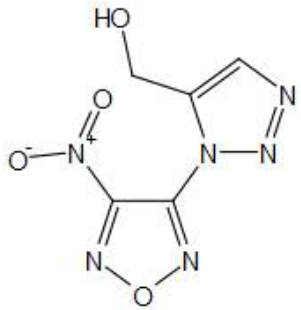
S3. Copies of NMR spectra


OH
O
N+
O-
N
N
N
N
N
O

3a

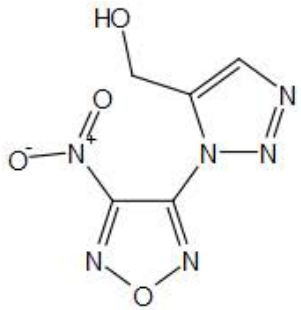
8.63
5.54
4.71
1.00
0.83
2.00
15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


155.92
149.74
146.03
125.91
55.01
OH
O
N
O
N
N
N
N
N
O
3a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


HO
O
N+
O-
N
N
N
N
N
O

3b

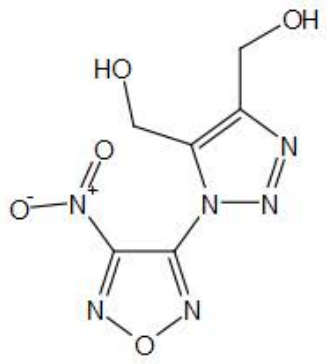
8.01
5.93
4.78
1.01
1.00
2.00
15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0



3b

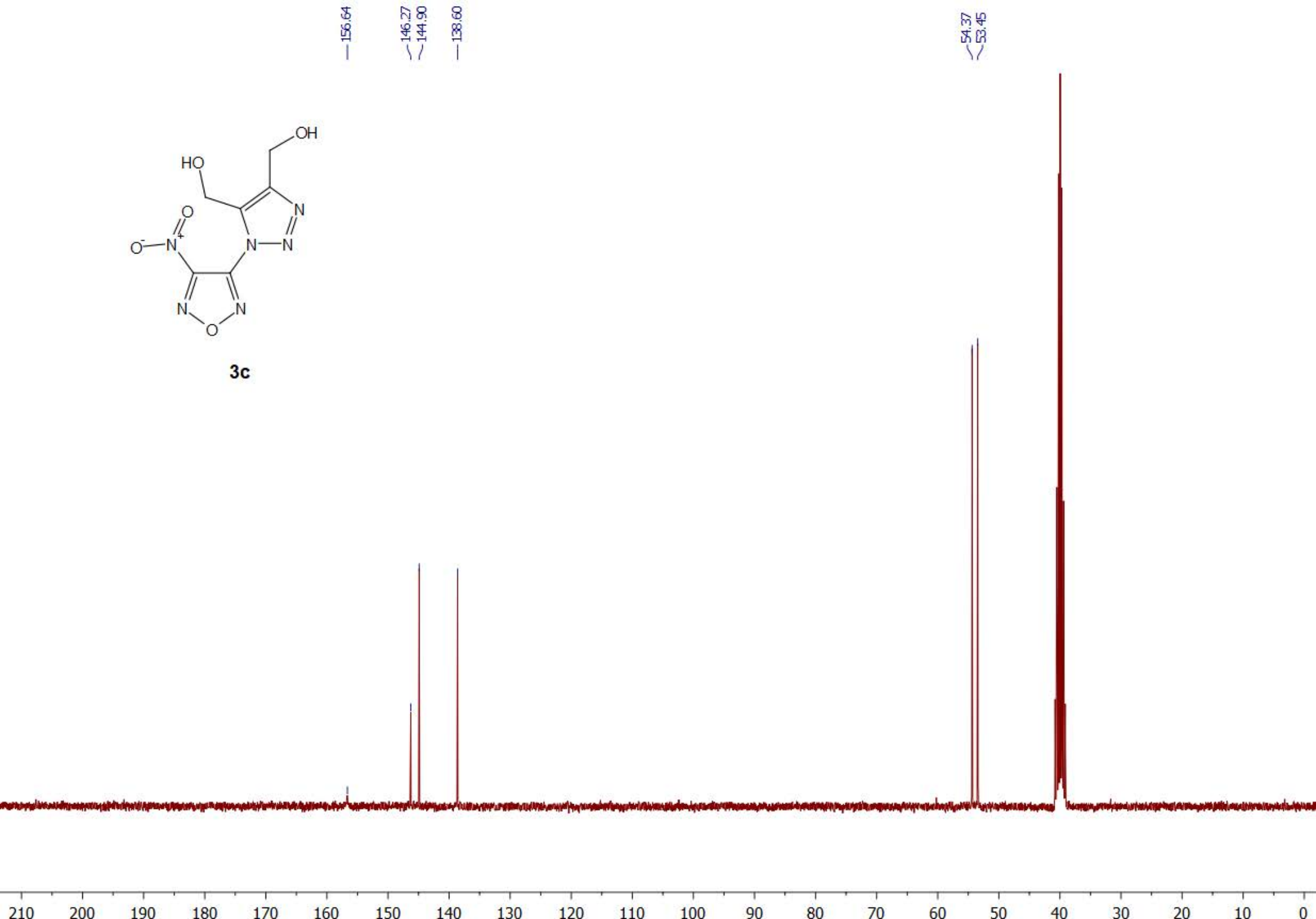
156.51
145.85
142.21
132.63
53.66

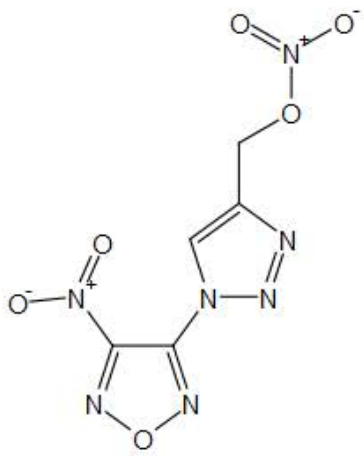
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


OH
HO
O
O-
N+
N
N
N
N
N
O

3c

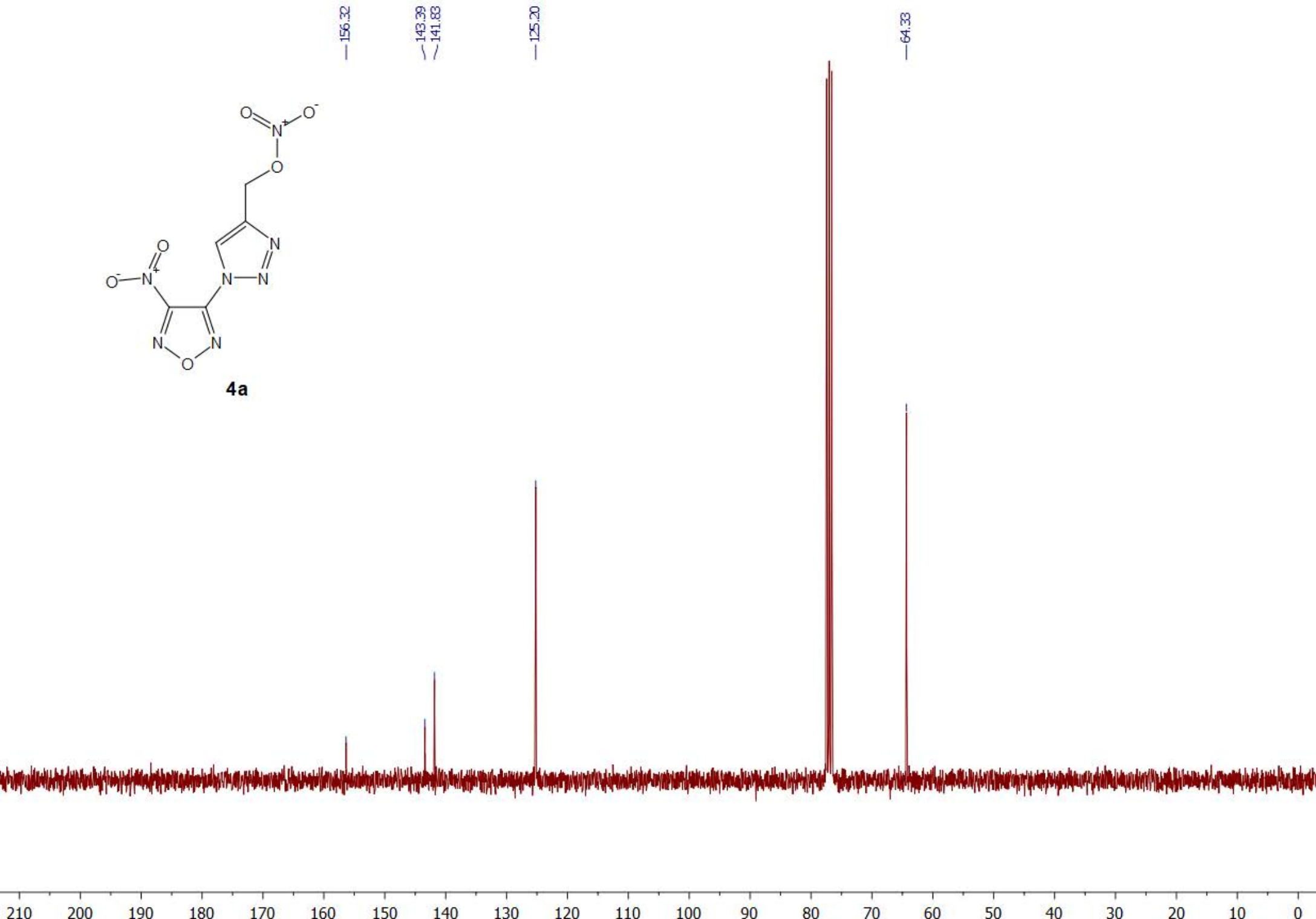
5.90
5.30
4.82
4.65
0.91
0.93
2.04
2.00
15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

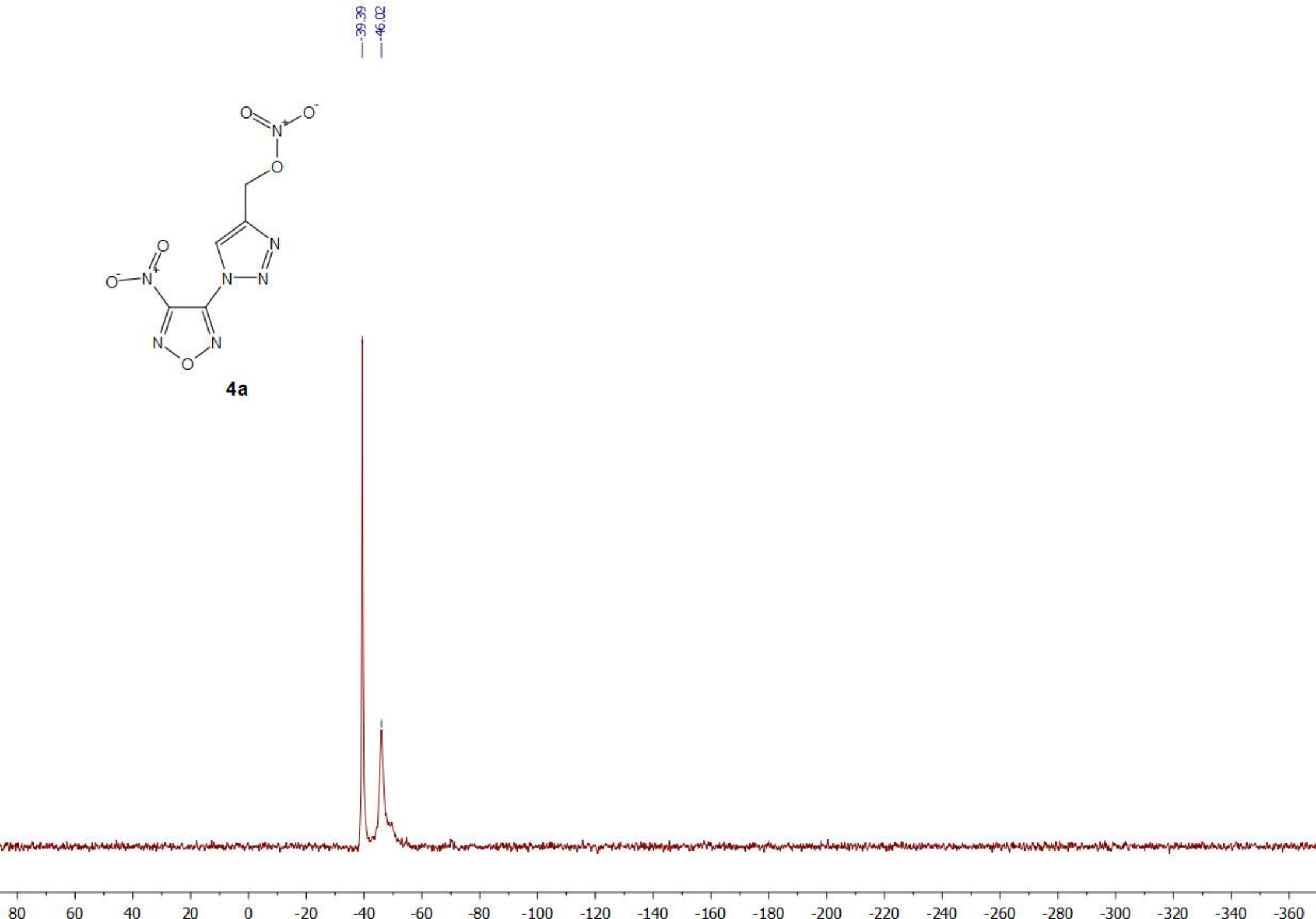

156.64
146.27
144.90
138.60
54.37
53.45
OH
HO
O
O-
N+
N
N
N
N
N
O
3c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

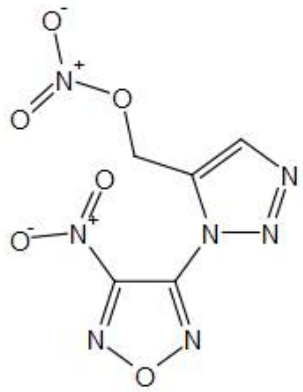


4a

8.47
5.73
1.00
2.00
15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 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 0.0


156.32
143.39
141.83
125.20
64.33
4a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


-39.39
-46.02
4a
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
-320
-340
-360



4b

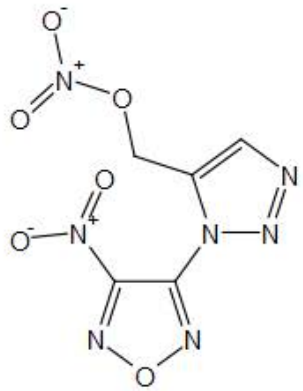
8.05

5.82

1.01

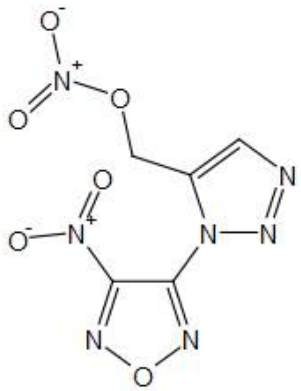
2.00

15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 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 0.0



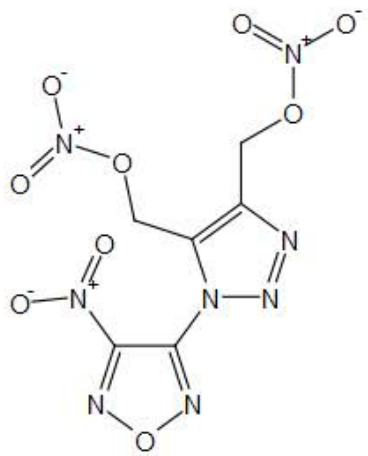
4b

154.04
143.23
136.56
131.99
60.61
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0



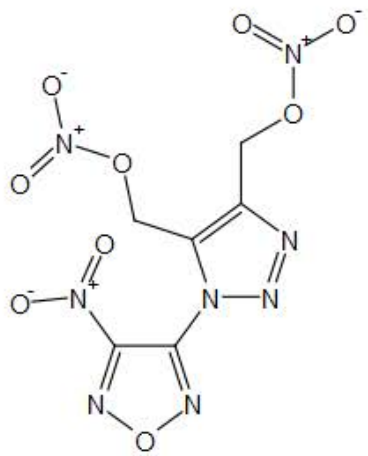
4b

-40.45
-50.34
80
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
-320
-340
-360



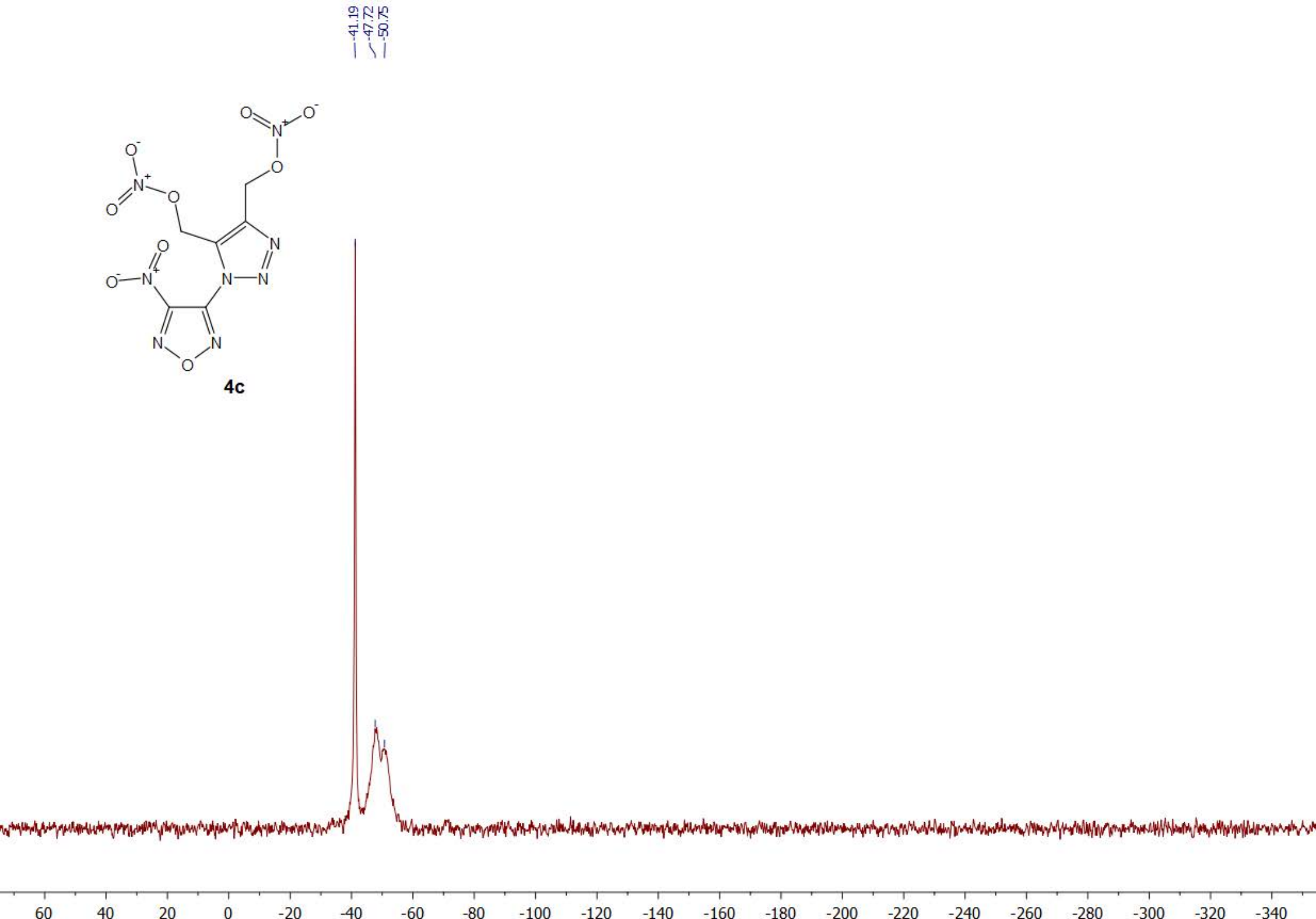
4c

5.87
5.76
2.00
1.98
15.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 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 0.0



4c

154.17
143.14
141.74
131.84
63.67
59.77
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


-41.19
-47.72
-50.75
4c
60
40
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-220
-240
-260
-280
-300
-320
-340