New Journal of Chemistry

Supporting Information for:

Methyl Sydnone Imine and Its Energetic Salts

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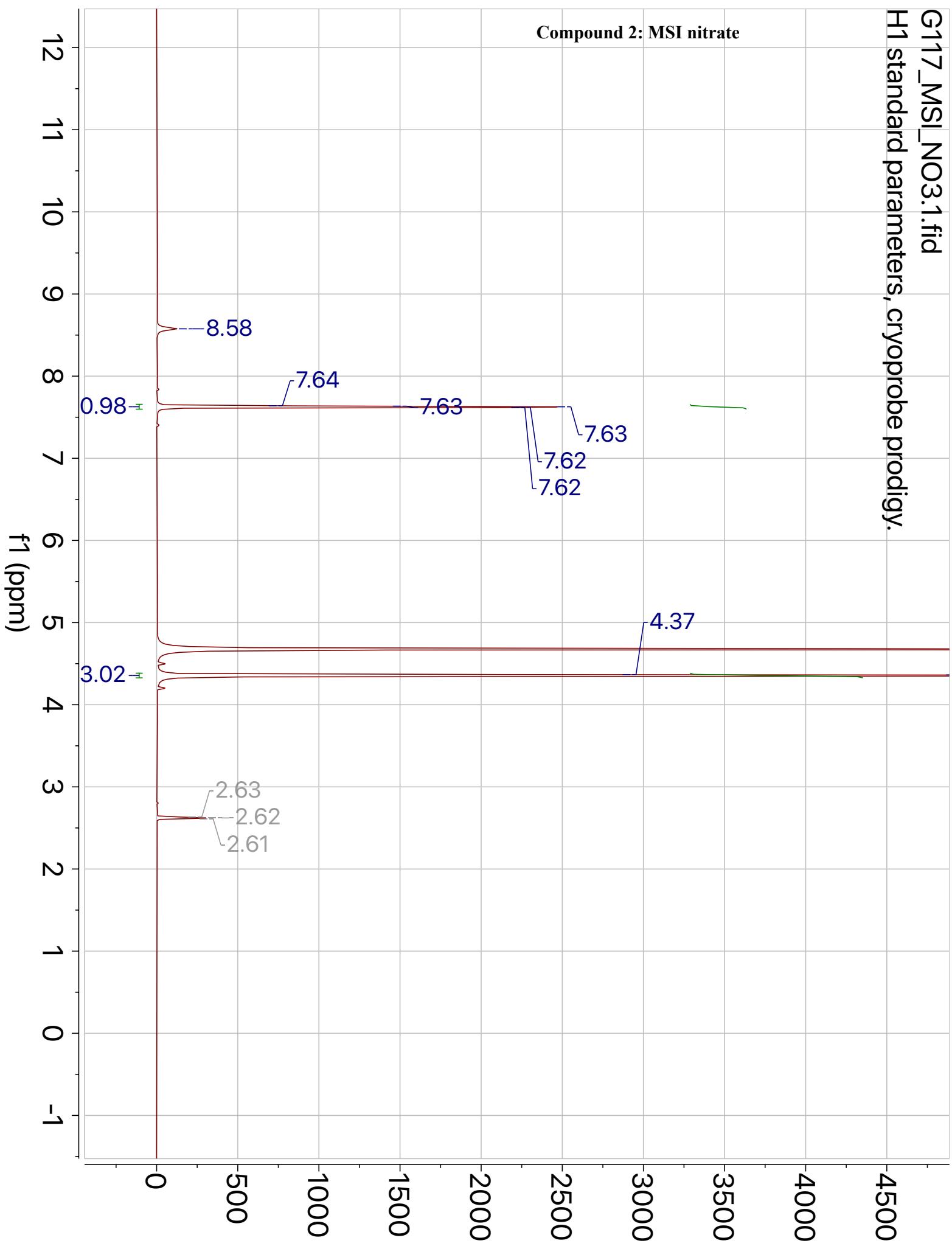
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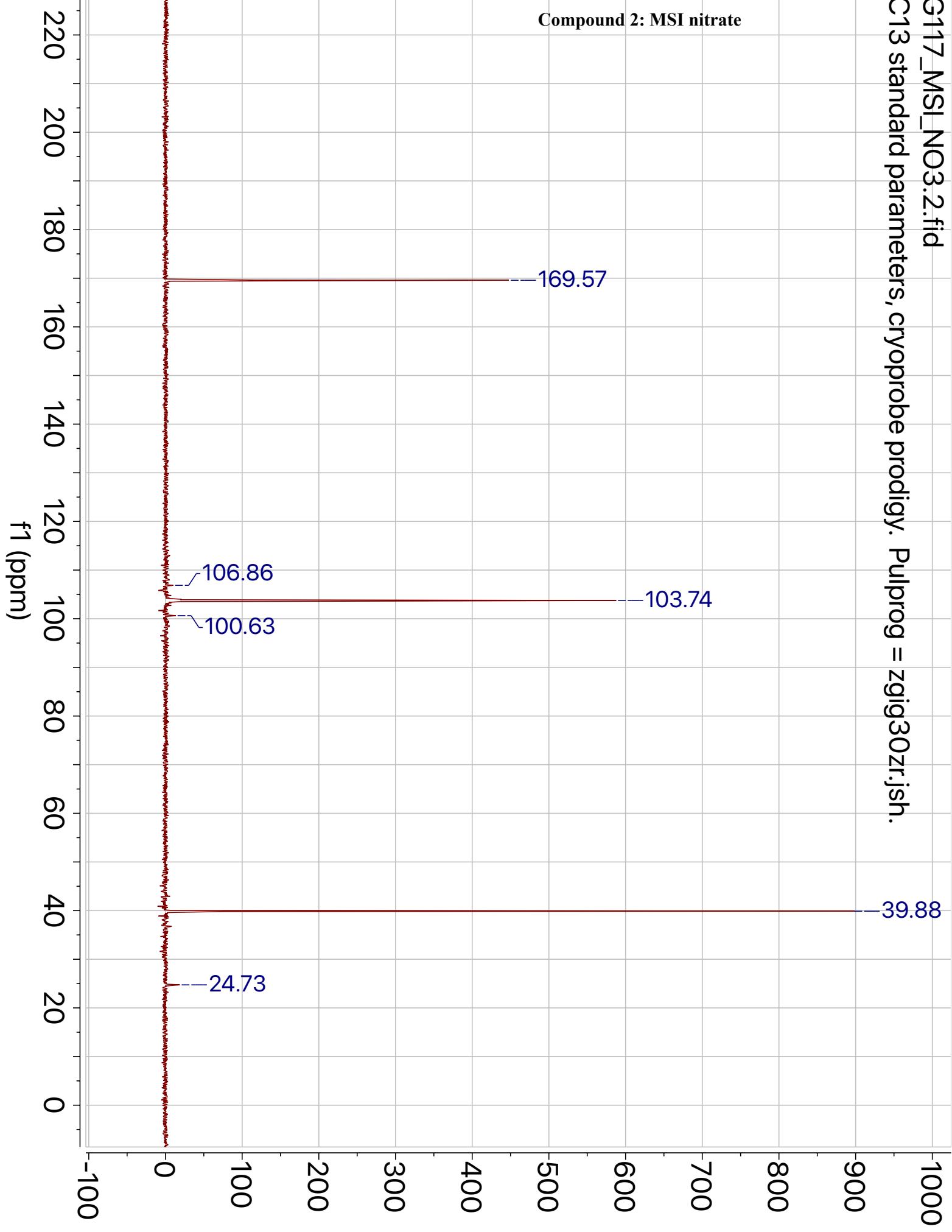
Compound 2: MSI nitrate
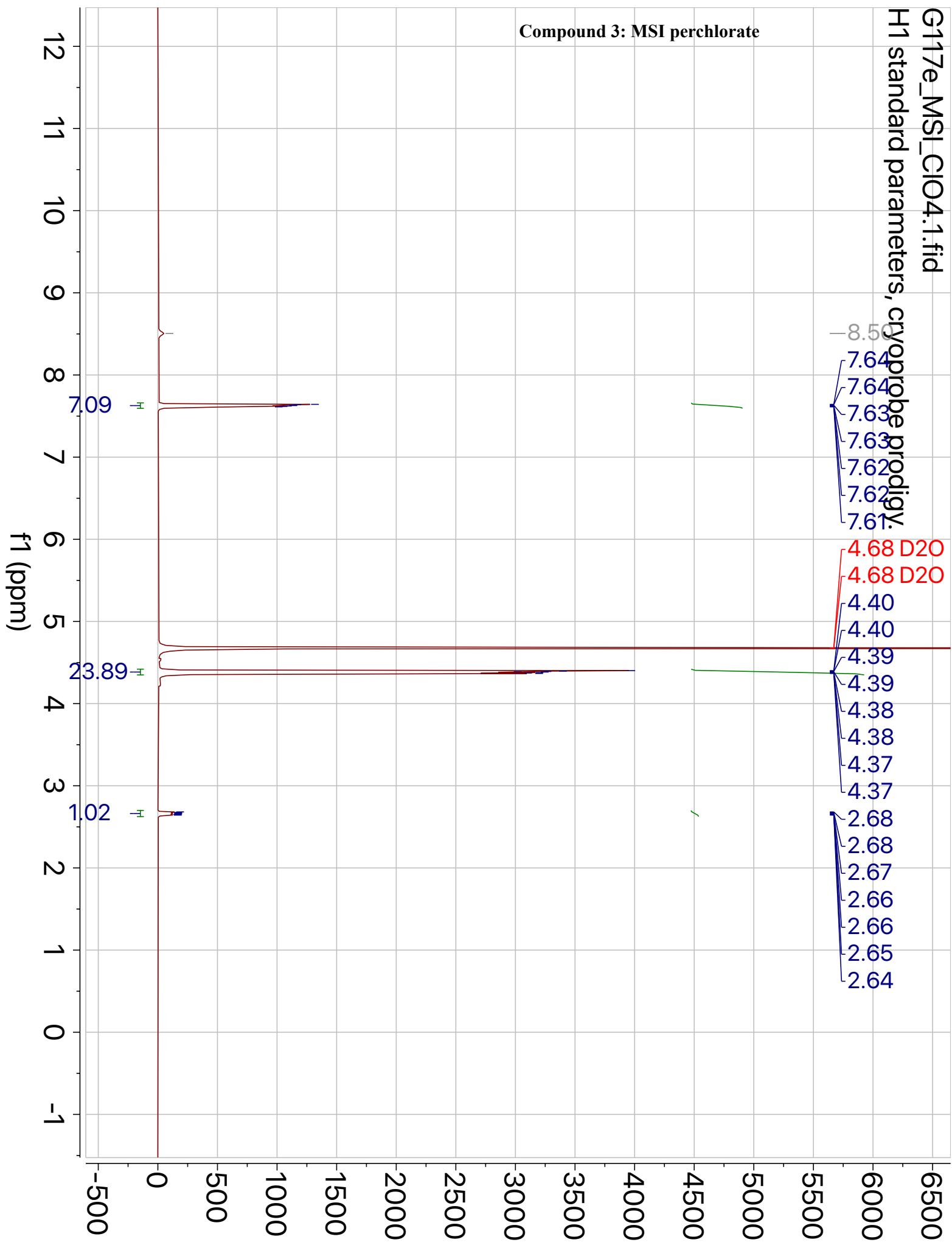
G117_MSI_NO3.1.fid
H1 standard parameters, cryoprobe prodigy.

G117_MSI_NO3.2.fid
C13 standard parameters, cryoprobe prodigy. Pulprog = zgig30zr.jsh.

Compound 2: MSI nitrate

169.57

106.86
103.74
100.63

39.88

24.73

Compound 3: MSI perchlorate

G117e_MSI_ClO4.1.fid
H1 standard parameters, cryoprobe prodigy.

—8.50
7.64
7.64
7.63
7.63
7.62
7.62
7.61
4.68 D2O
4.68 D2O
4.40
4.40
4.39
4.39
4.38
4.38
4.37
4.37
2.68
2.68
2.67
2.66
2.66
2.65
2.64

7.09
23.89
1.02

f1 (ppm)

Compound 3: MSI perchlorate

169.59

103.91

39.99

24.87

f1 (ppm)

Compound 4: MSI nitrotetrazole

1.02 — 8.62

1.92 — 7.50
7.50

20.05 — 4.68

4.22 D2O

2.60
2.59

f1 (ppm)
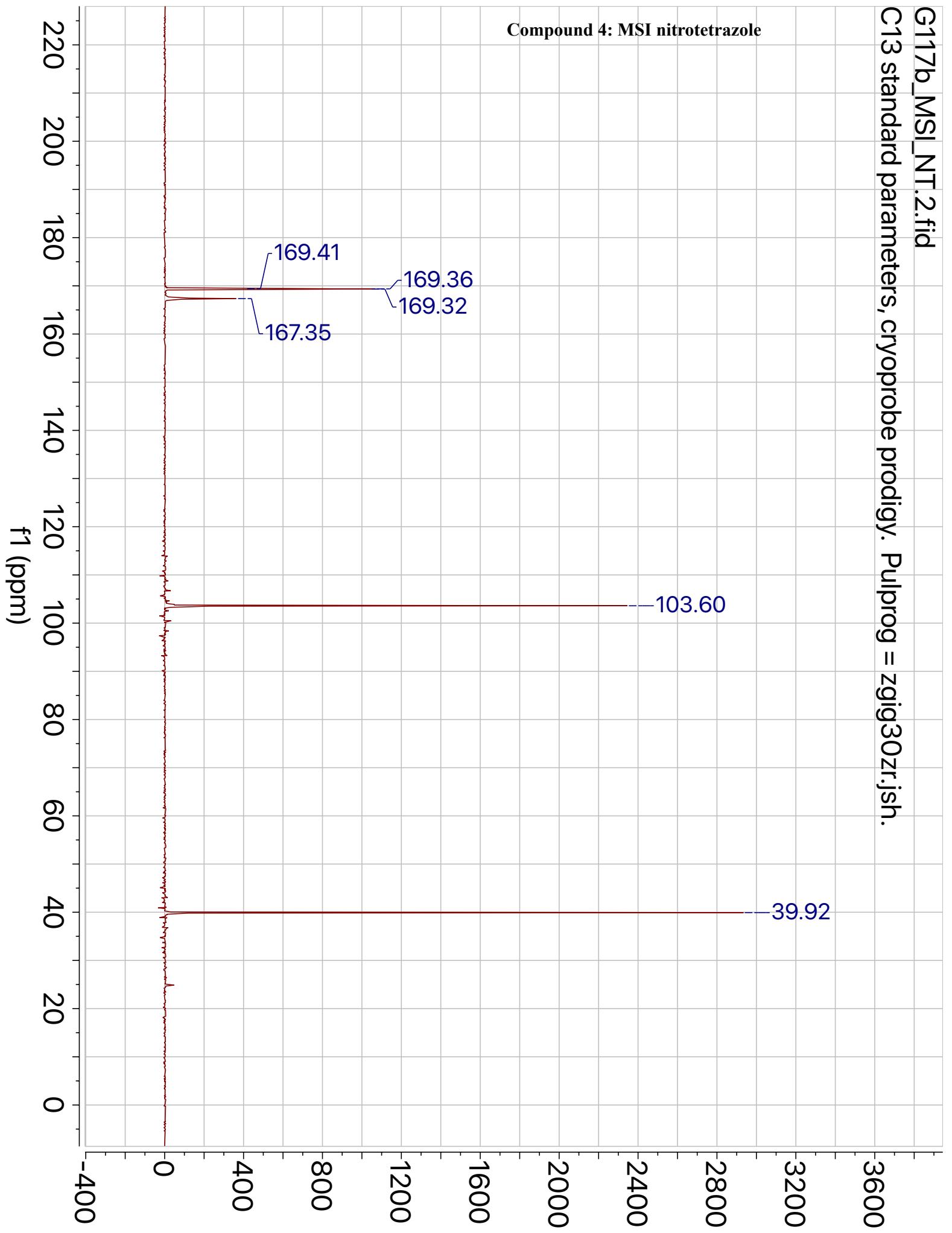
Compound 4: MSI nitrotetrazole

G117b_MSI_NT.2.fid
C13 standard parameters, cryoprobe prodigy. Pulprog = zgig30zr.jsh.

169.41
169.36
169.32
167.35
103.60
39.92

f1 (ppm)
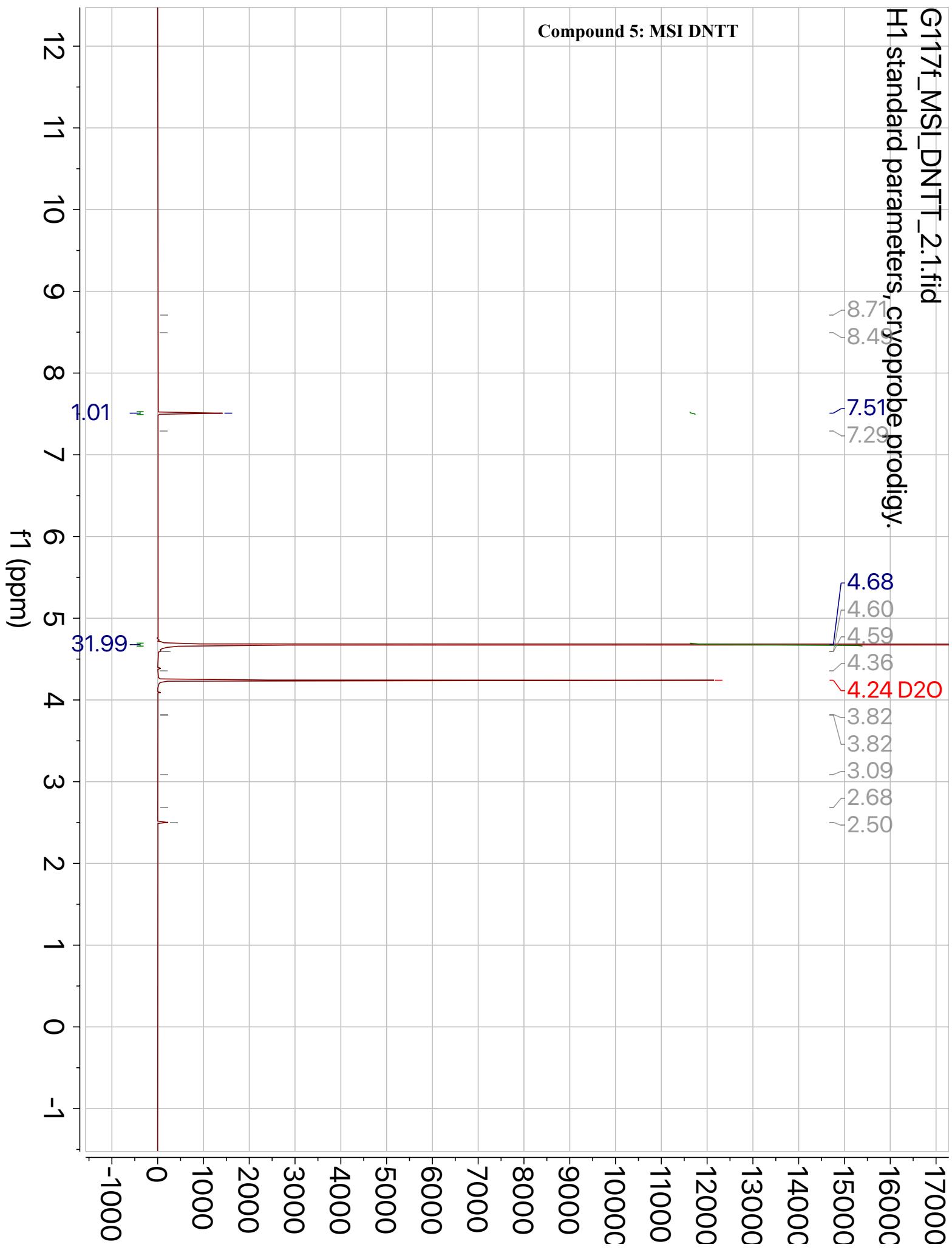
Compound 5: MSI DNTT

G117f_MSI_DNTT_2.1.fid
H1 standard parameters, cryoprobe prodigy.

8.71
8.49
7.51
7.29

4.68
4.60
4.59
4.36
4.24 D2O
3.82
3.82
3.09
2.68
2.50

1.01
31.99

f1 (ppm)

Compound 5: MSI DNTT

- 169.44
- 164.31
- 161.75
- 142.76
- 103.47
- 39.73
- 39.70

f1 (ppm)

Compound 6: MSI Tetrazole Azasydnone

f1 (ppm)

8.64
8.55
8.11
7.98
1.03
7.51
7.51
7.50
7.29
5.21
5.21
4.47
4.47
4.67
22.96
4.23 D2O
3.78
3.78
3.03
2.54
2.54
1.03
1.86
1.85
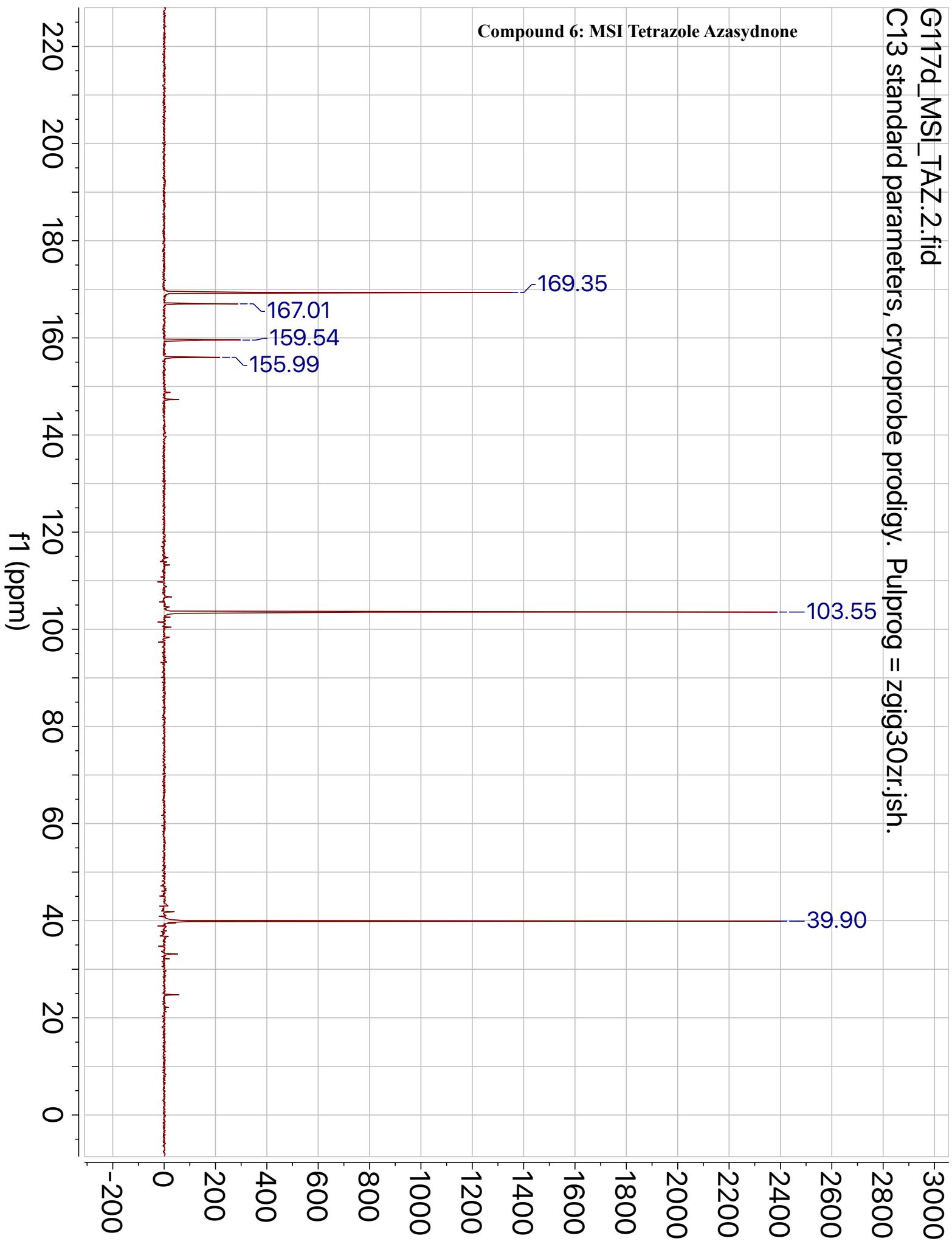
G117d_MSI_TAZ.2.fid

C13 standard parameters, cryoprobe prodigy. Pulprog = zgig30zr.jsh.

Compound 6: MSI Tetrazole Azasydnone

169.35

167.01

159.54

155.99

103.55

39.90

f1 (ppm)

G117c4_MSI_NO2BF4_1.1.fid
H1 standard parameters, cryoprobe prodigy.

Compound 8: 3-methyl-1,2,3-oxadiazolium nitrosoamide

8.07
8.06
6.32
5.18
5.18
5.17
4.41
4.41
4.40
4.30
4.29
4.29
4.28
3.99
3.99
3.98
3.86
3.86
3.85
3.27
3.27
3.26
3.07
3.07
3.06 H2O
2.89
1.98
1.96
1.96 CD3CN
1.95 CD3CN
1.95 CD3CN
1.94 CD3CN
1.94 CD3CN
1.93
1.93
1.92
1.91
1.91
1.89
1.89
1.27

2.02
7.13
0.99
10.04
6.67
10.15

f1 (ppm)
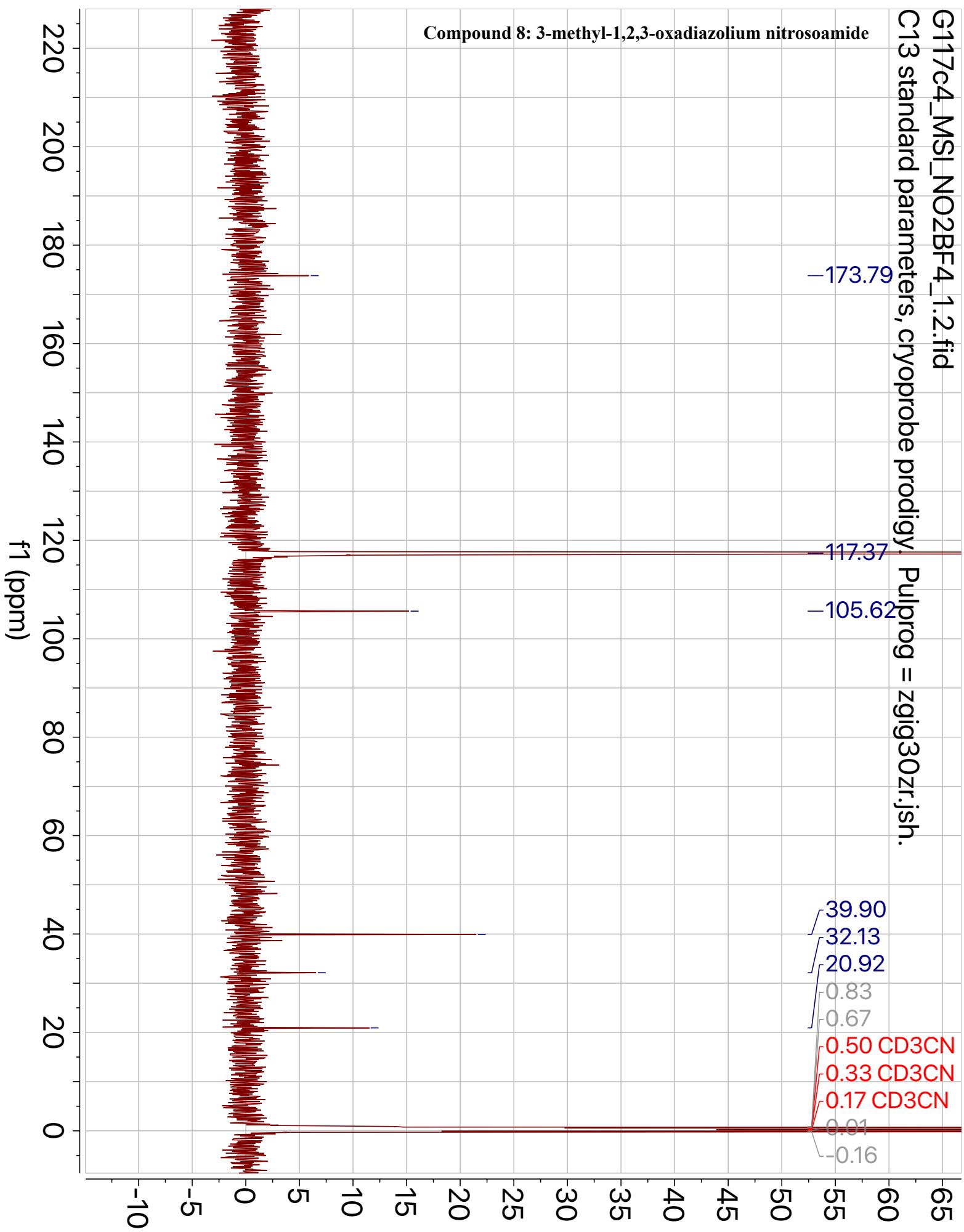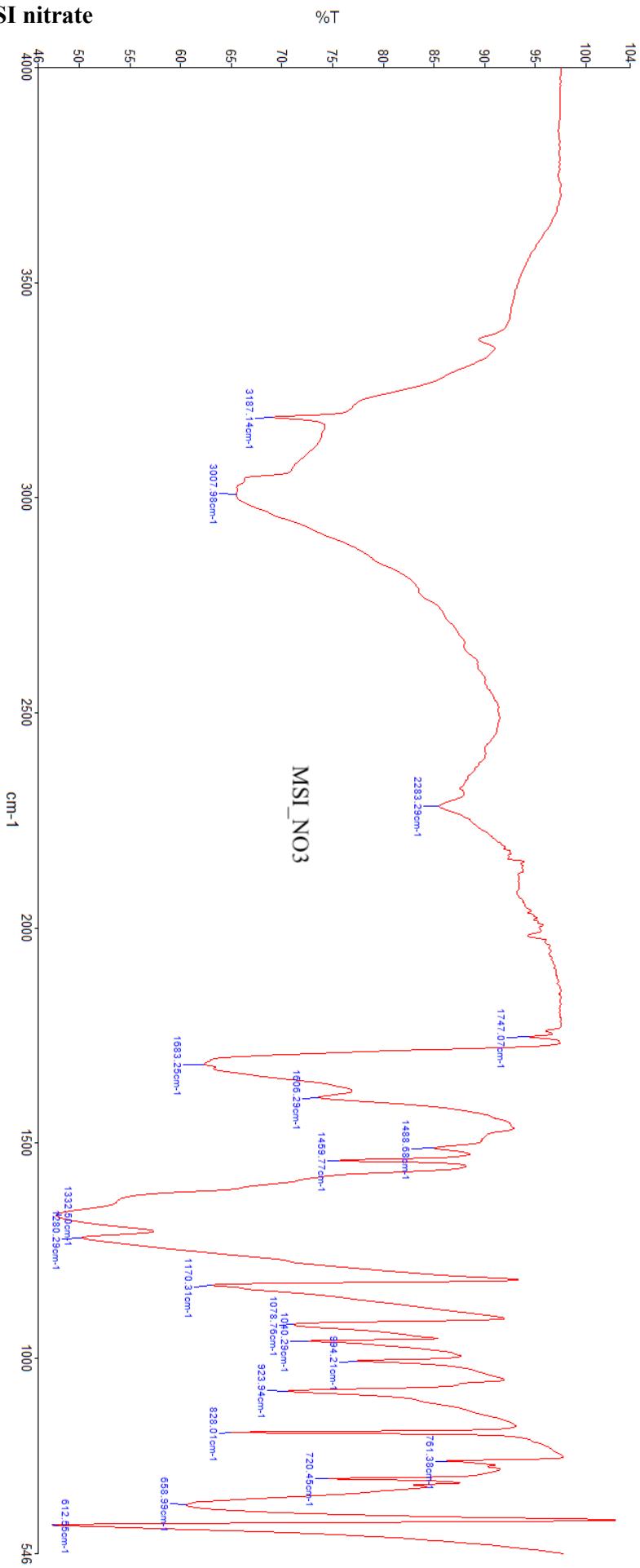
G117c4_MSI_NO2BF4_1.2.fid
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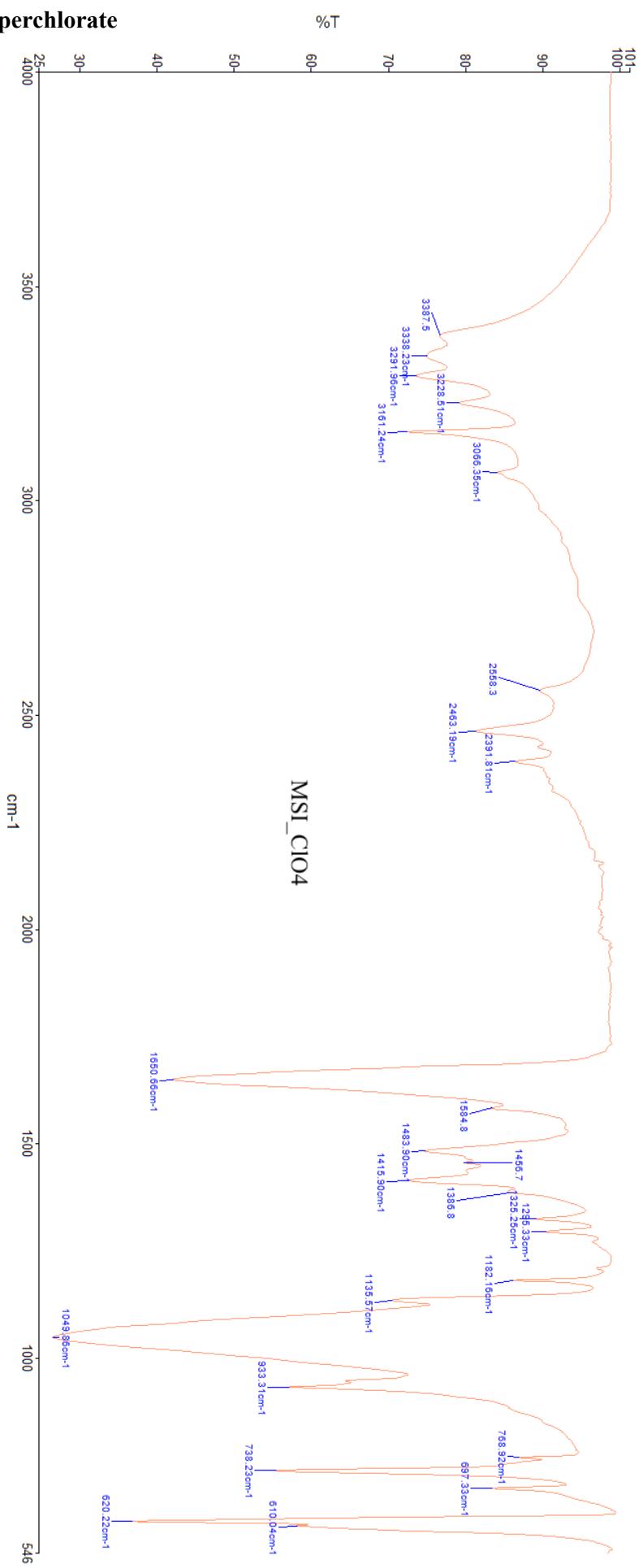
Compound 8: 3-methyl-1,2,3-oxadiazolium nitrosoamide

—173.79
—117.37
—105.62
39.90
32.13
20.92
0.83
0.67
0.50 CD3CN
0.33 CD3CN
0.17 CD3CN
0.01
—0.16

f1 (ppm)

Compound 2: MSI nitrate

%T

MSI_NO3

cm-1

3187.14cm-1
307.98cm-1
2283.29cm-1
1747.07cm-1
1683.25cm-1
1606.29cm-1
1459.77cm-1
1488.68cm-1
1332.55cm-1
1280.29cm-1
1170.31cm-1
1078.76cm-1
1040.29cm-1
984.21cm-1
923.94cm-1
828.01cm-1
761.38cm-1
720.46cm-1
658.99cm-1
612.55cm-1
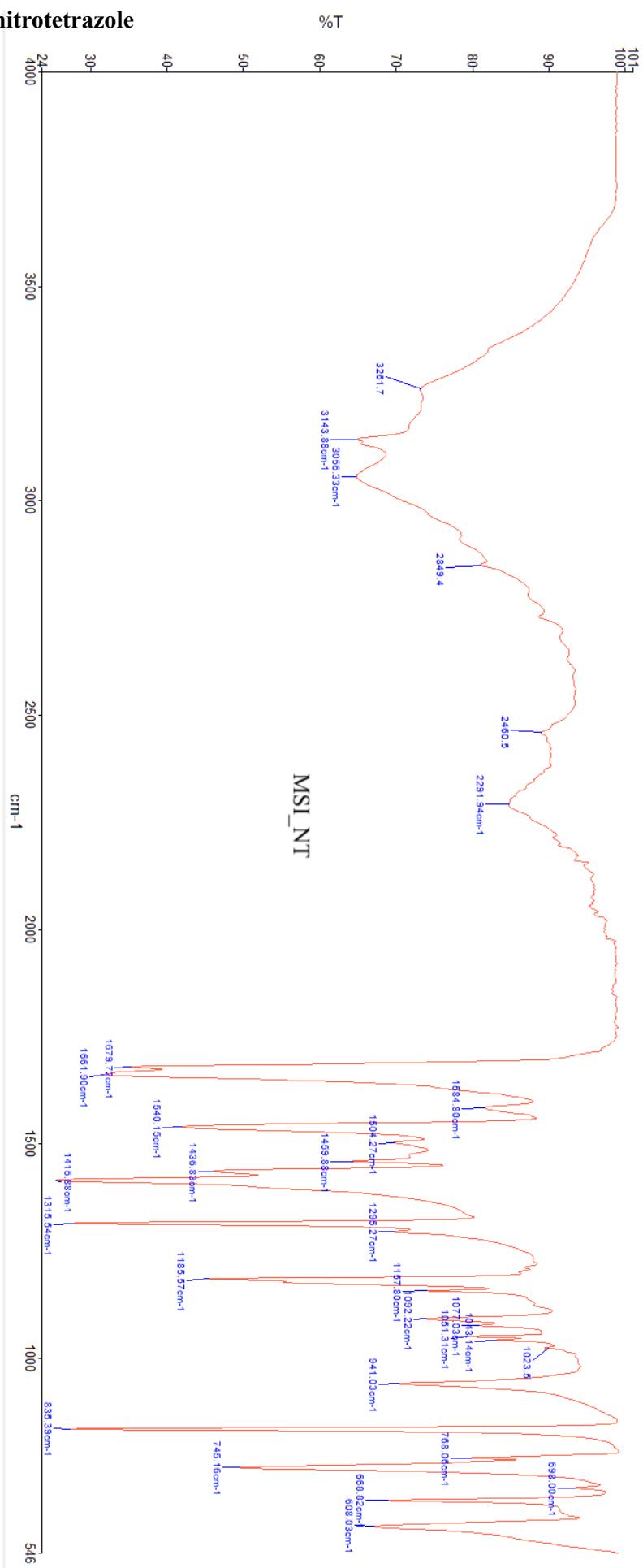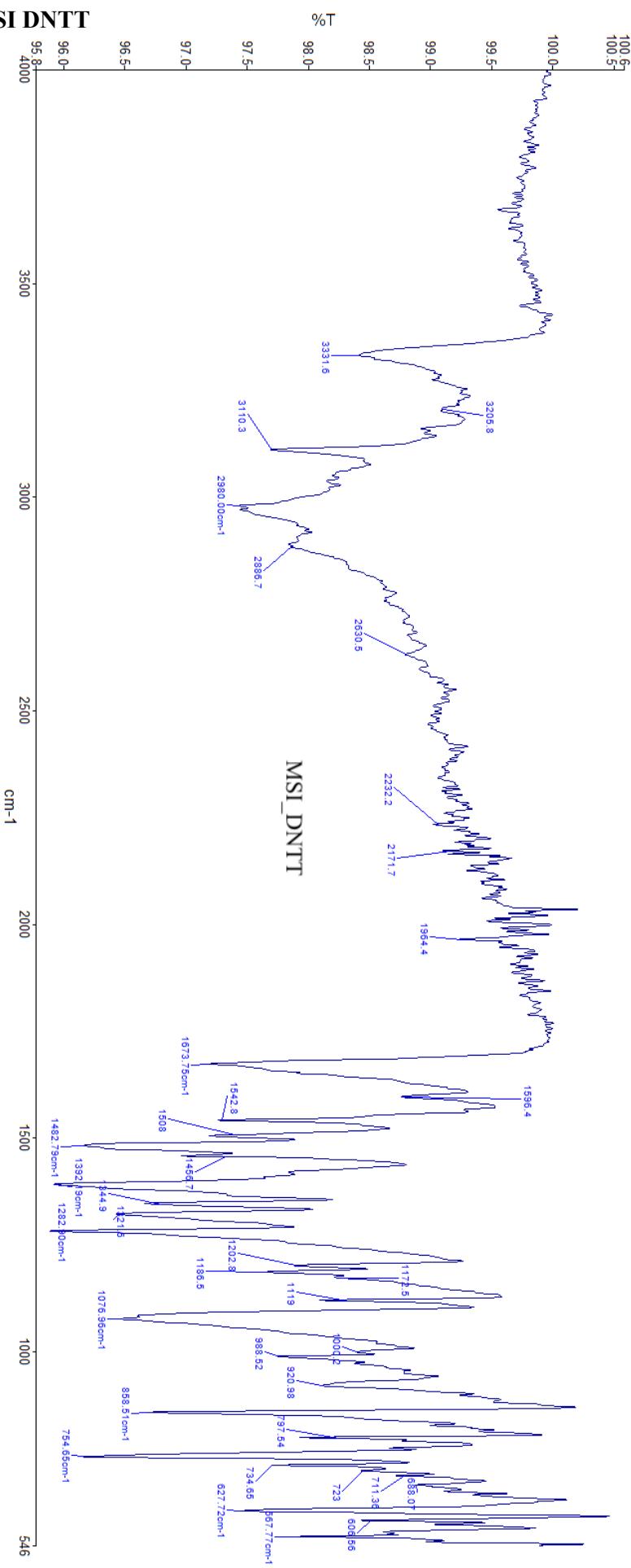
Compound 3: MSI perchlorate

Compound 4: MSI nitrotetrazole

%T

MSI_NT
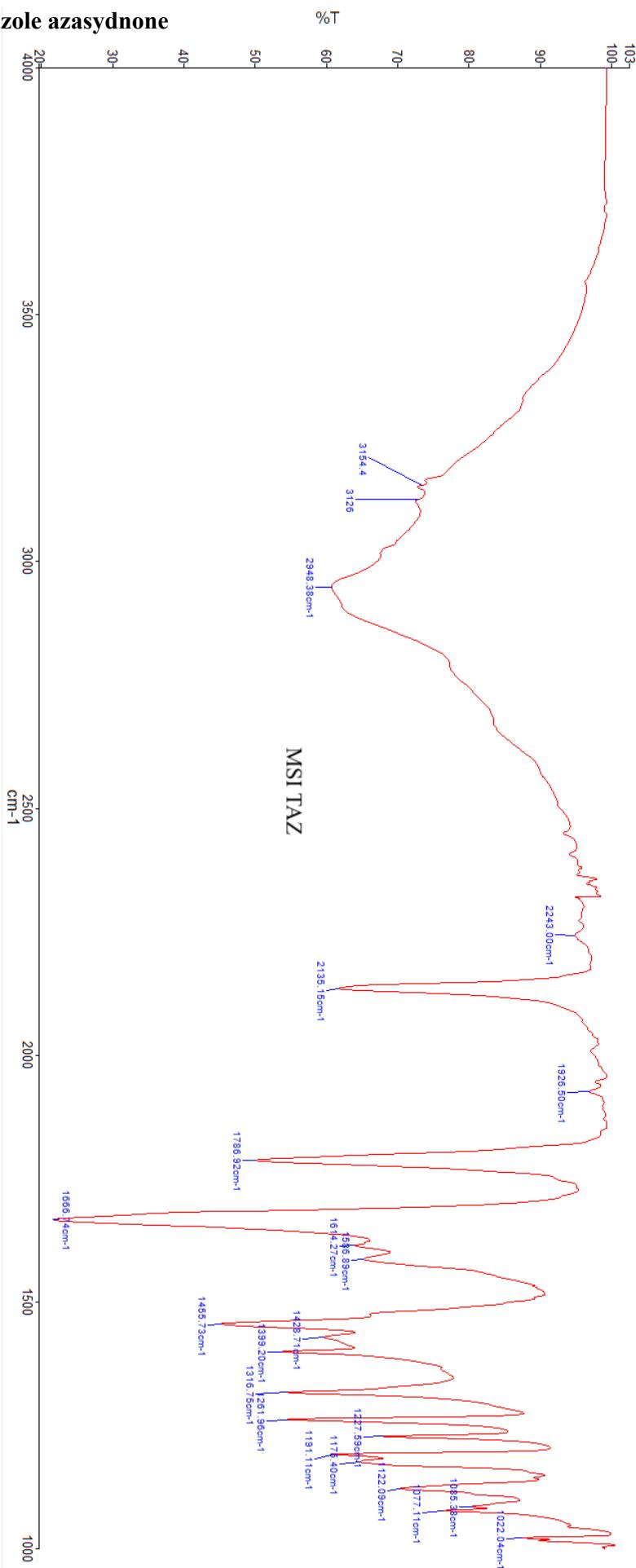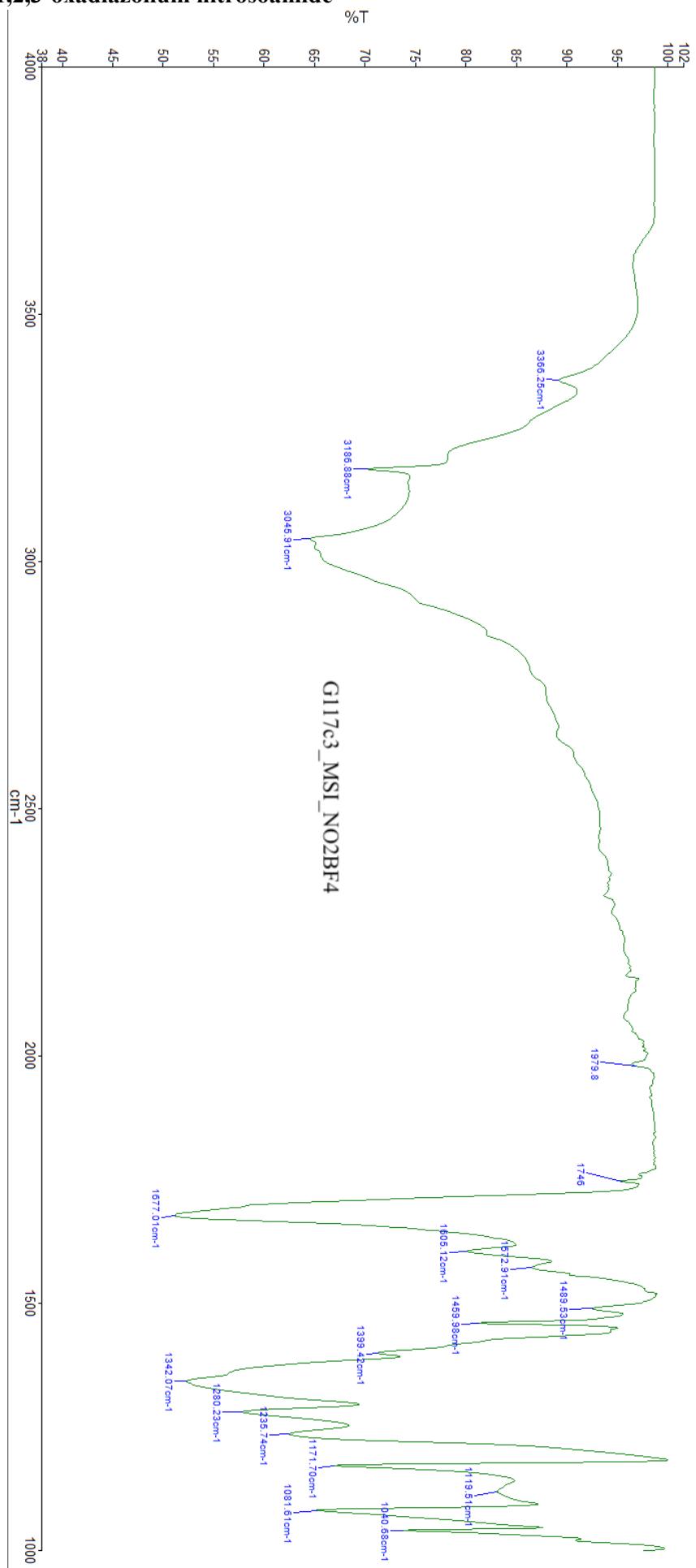
Compound 5: MSI DNTT

MSI_DNTT

Compound 6: MSI tetrazole azasydnone
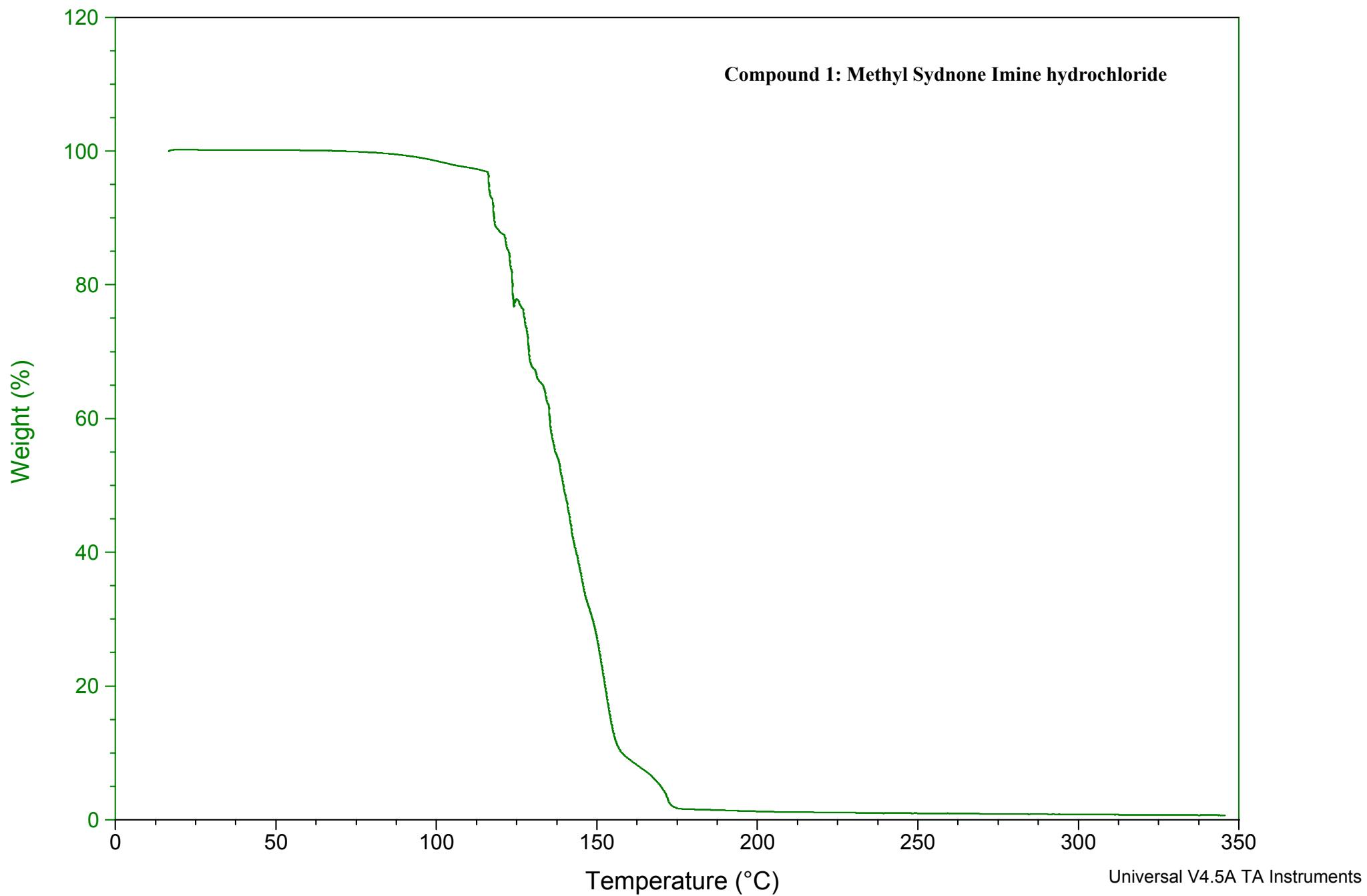
MSI TAZ

Compound 8: 3-methyl-1,2,3-oxadiazolium nitrosoamide
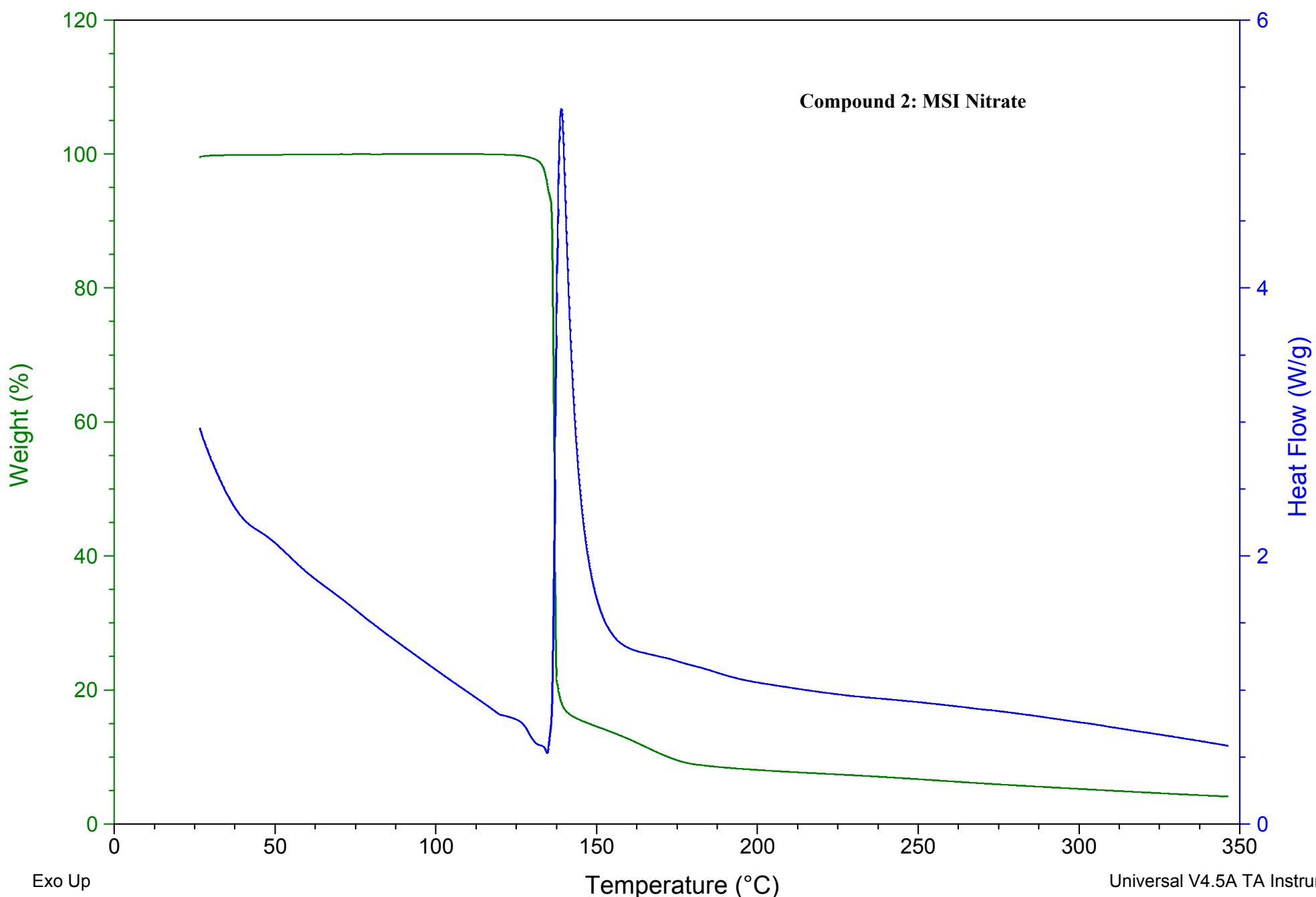
DSC-TGA

Sample: G117_MSI_NO3
Size: 3.7690 mg
Method: Gettings Sample Analysis 5Cmin
Comment: 3.83 mg sample
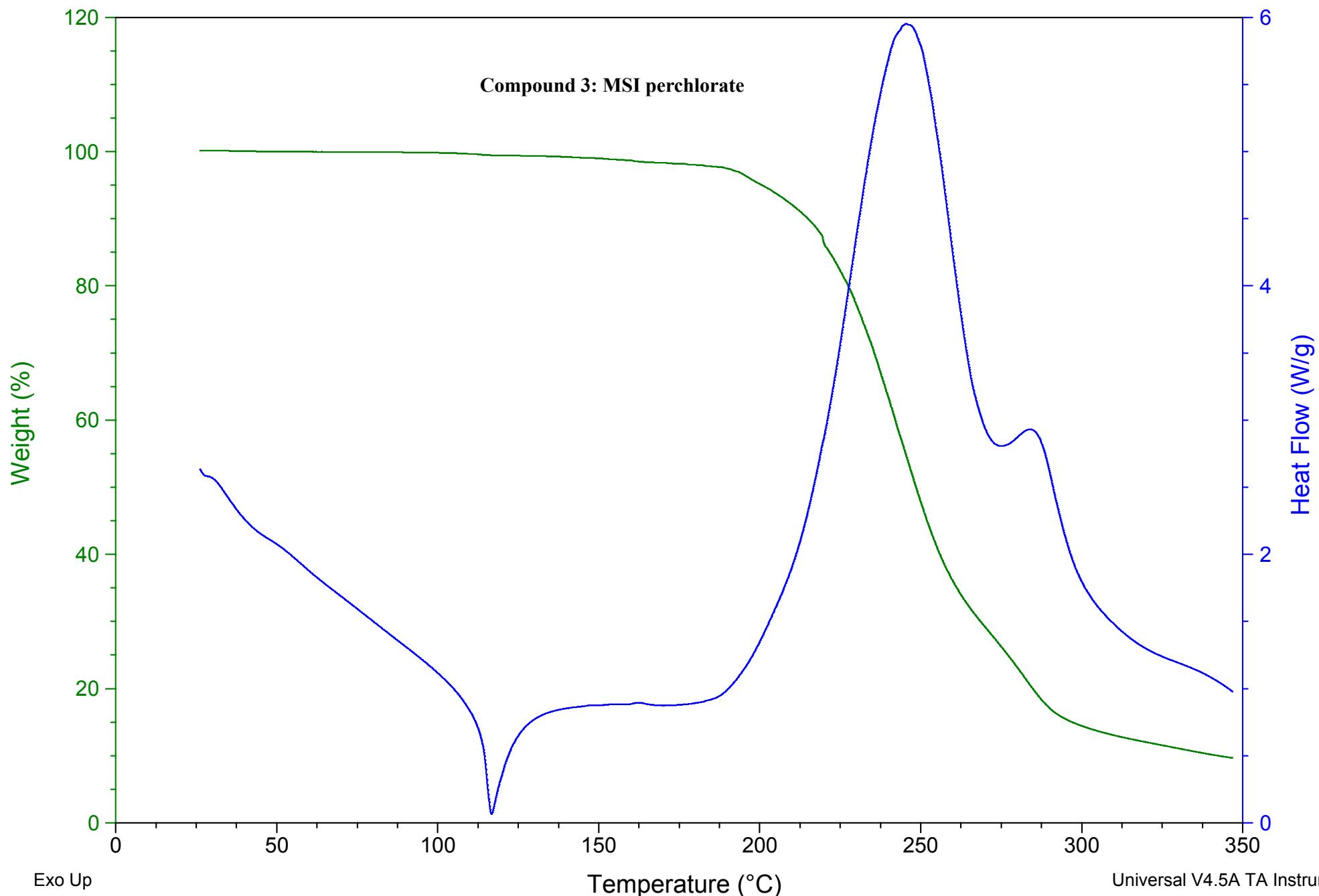
File: C:...\SDT\Gettings\MSI\G117_MSI_NO3.002
Operator: MG
Run Date: 19-Aug-2020 14:59
Instrument: SDT Q600 V20.9 Build 20

Compound 2: MSI Nitrate

Exo Up

Universal V4.5A TA Instruments

DSC-TGA

Sample: G117_MSI_ClO4
Size: 3.7850 mg
Method: Gettings Sample Analysis 5Cmin
Comment: 3.7 mg sample
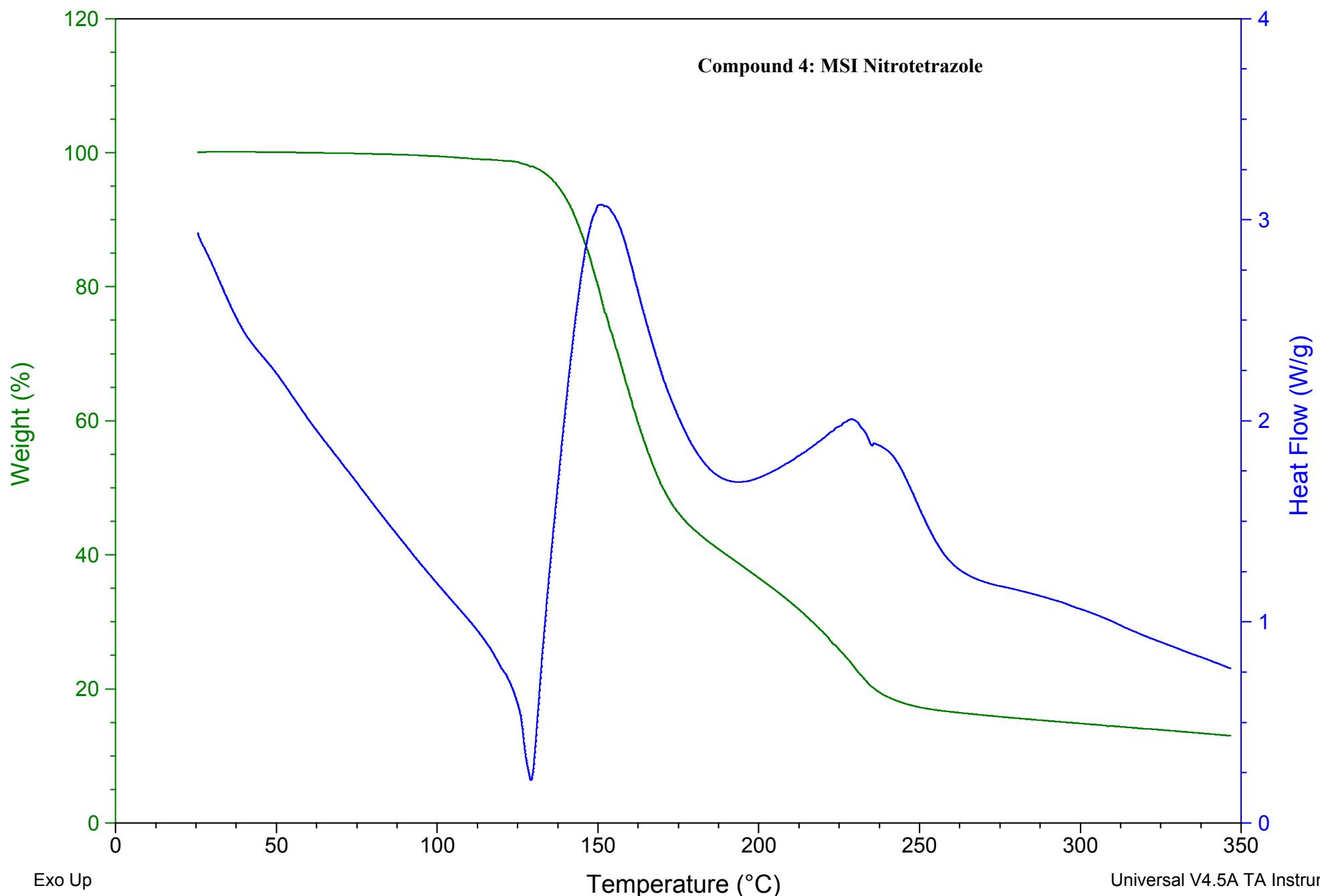
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Operator: MG
Run Date: 19-Aug-2020 19:10
Instrument: SDT Q600 V20.9 Build 20

Compound 3: MSI perchlorate

Exo Up

Universal V4.5A TA Instruments

DSC-TGA

Sample: G117_MSI_NT
Size: 3.6250 mg
Method: Gettings Sample Analysis 5Cmin
Comment: 3.95 mg sample
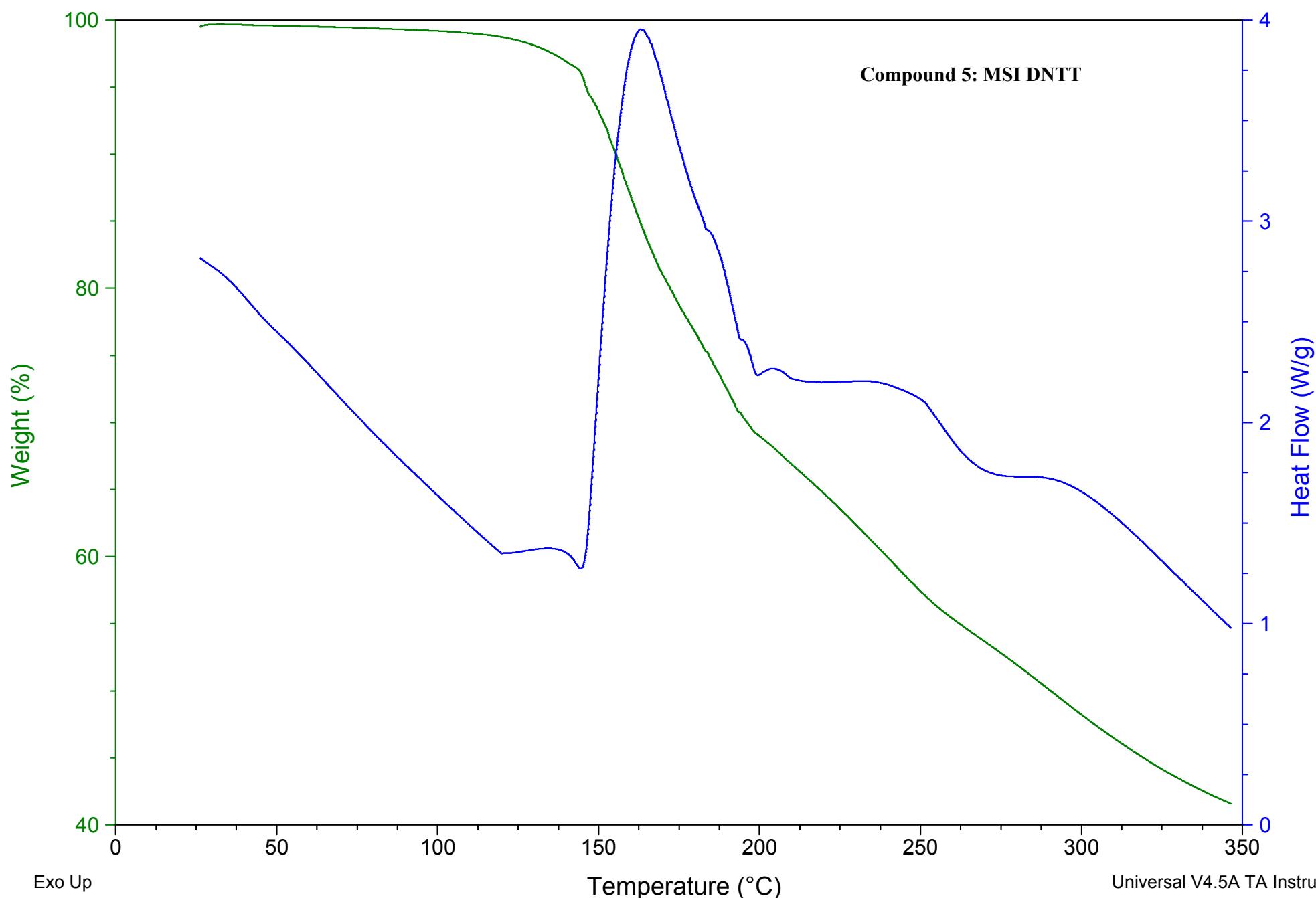
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Operator: MG
Run Date: 19-Aug-2020 13:37
Instrument: SDT Q600 V20.9 Build 20

Compound 4: MSI Nitrotetrazole

Exo Up

Universal V4.5A TA Instruments

Sample: G117_MSI_DNTT
Size: 4.0800 mg
Method: Gettings Sample Analysis 5Cmin
Comment: 3.94 mg sample

DSC-TGA
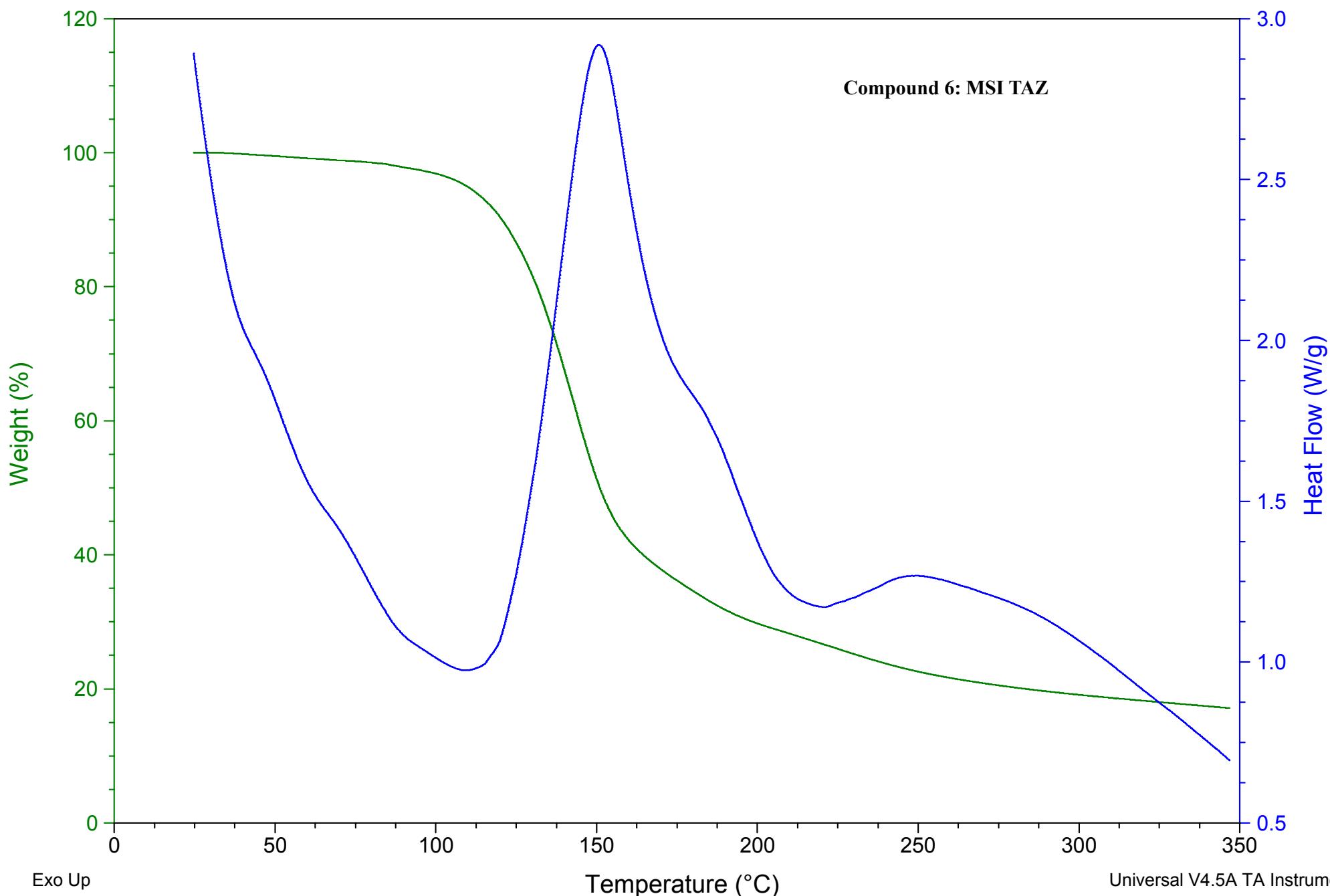
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Operator: MG
Run Date: 19-Aug-2020 11:35
Instrument: SDT Q600 V20.9 Build 20

Compound 5: MSI DNTT

Exo Up

Universal V4.5A TA Instruments
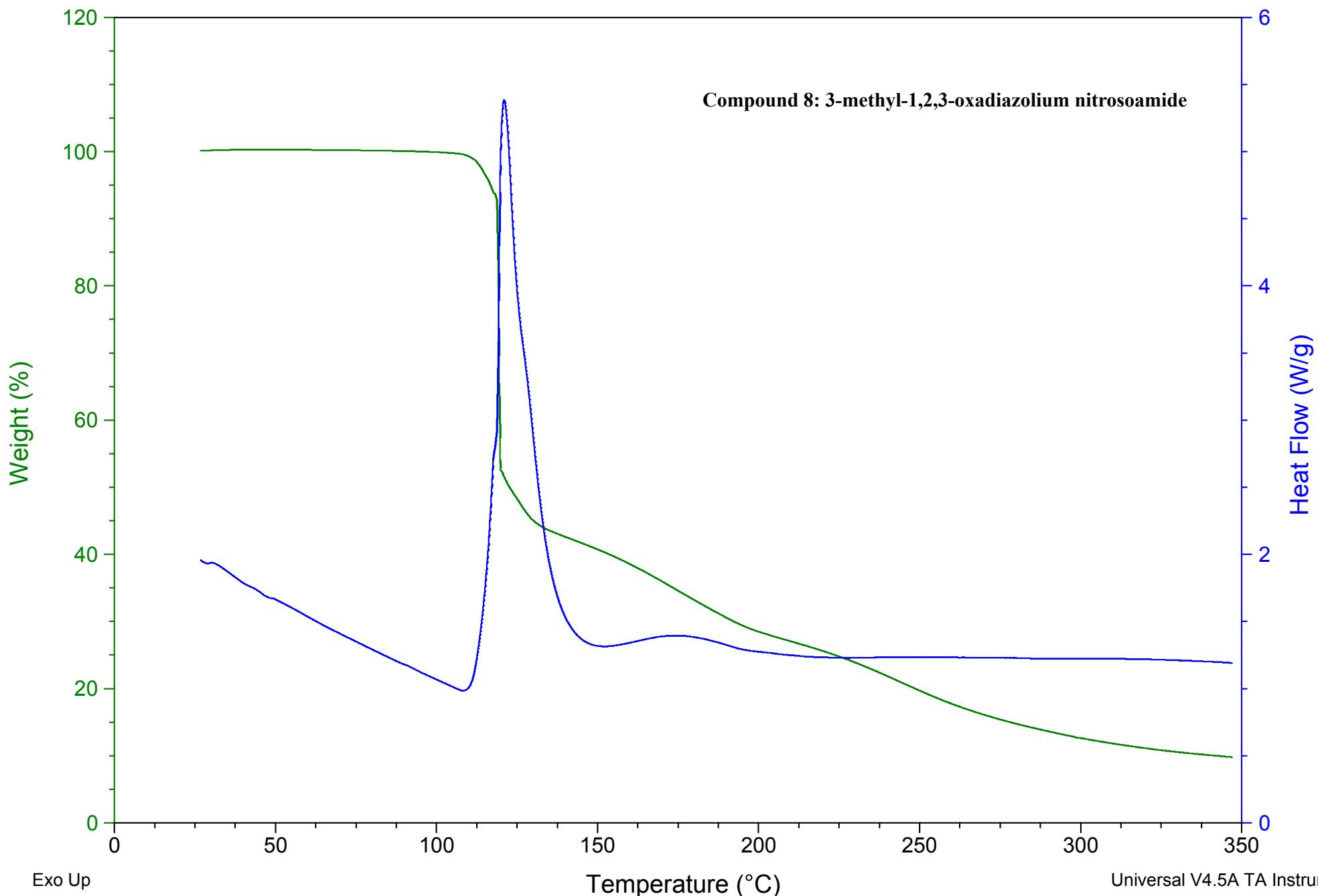
DSC-TGA

Sample: MSI_NO2BF4
Size: 5.3020 mg
Method: Gettings Sample Analysis 5Cmin
Comment: 4.9 mg sample

File: C:...\Gettings\MSI\G117c_MSI_NO2BF4.001
Operator: MG
Run Date: 23-Sep-2020 17:43
Instrument: SDT Q600 V20.9 Build 20

Compound 8: 3-methyl-1,2,3-oxadiazolium nitrosoamide

Exo Up

Universal V4.5A TA Instruments

Compound 2
CCDC-2024994

Fig. 1 Molecular unit of 5-amino-3-methyl-1,2,3-oxadiazolium nitrate (**2**). Ellipsoids are drawn at the 50% probability level. Disorder of methyl H atoms is symmetry imposed by a mirror plane bisecting the cation.

Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$C_3H_6N_3O \cdot NO_3$
M_r	162.12
Crystal system, space group	Monoclinic, $P2_1/m$
Temperature (K)	150
a, b, c (Å)	5.7481 (6), 5.8420 (7), 9.9504 (11)
β (°)	91.390 (5)
V (Å^3)	334.04 (6)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.31
Crystal size (mm)	$0.15 \times 0.13 \times 0.09$
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating and photon counting pixel array detector
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.633, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2988, 764, 711
R_{int}	0.033
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.637
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.105, 1.15
No. of reflections	764
No. of parameters	72
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.29

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

Table 2

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3—H3$A\cdots$O3	0.90 (3)	1.90 (3)	2.806 (2)	180 (2)
N3—H3$B\cdots$O2[i]	0.87 (3)	2.06 (3)	2.905 (2)	162 (2)
N3—H3$B\cdots$O3[i]	0.87 (3)	2.39 (3)	3.114 (2)	141 (2)
C1—H1$\cdots$O3[i]	0.95	2.36	3.039 (2)	128
C3—H3$C\cdots$O2[ii]	0.98	2.37	3.260 (3)	150

Symmetry codes: (i) $x-1$, y, z; (ii) $x-1$, y, $z-1$.

References

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). J. Appl. Cryst., 37, 335–338.

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Sheldrick, G. M. (2015). "*SHELXT*–Integrated space-group and crystal-structure determination", Acta Cryst. A71, 3-8.

Sheldrick, G. M. (2018). *SHELXL2018*. University of Göttingen, Germany.

Spek, A. L. (2003). J. Appl. Cryst., 36, 7–13.

Figure 1

supporting information

Title

Computing details

Data collection: Apex3 v2019.1-0 (Bruker, 2019); cell refinement: *SAINT* V8.40A (Bruker, 2019); data reduction: *SAINT* V8.40A (Bruker, 2019); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

(G117_MSI_NO3_0m)

Crystal data

$C_3H_6N_3O·NO_3$	$F(000) = 168$
$M_r = 162.12$	$D_x = 1.612$ Mg m^{-3}
Monoclinic, $P2_1/m$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 5.7481$ (6) Å	Cell parameters from 2359 reflections
$b = 5.8420$ (7) Å	$\theta = 7.7–79.0°$
$c = 9.9504$ (11) Å	$\mu = 1.31$ mm^{-1}
$\beta = 91.390$ (5)°	$T = 150$ K
$V = 334.04$ (6) Å^3	Block, colourless
$Z = 2$	$0.15 \times 0.13 \times 0.09$ mm

Data collection

Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating and photon counting pixel array detector	Absorption correction: multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
Radiation source: I-mu-S microsource X-ray tube	$T_{min} = 0.633$, $T_{max} = 0.754$
Laterally graded multilayer (Goebel) mirror monochromator	2988 measured reflections
Detector resolution: 7.4074 pixels mm^{-1}	764 independent reflections
ω and phi scans	711 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.033$
	$\theta_{max} = 79.3°$, $\theta_{min} = 7.7°$
	$h = -7\rightarrow6$
	$k = -7\rightarrow7$
	$l = -12\rightarrow12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.105$	$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.0917P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.15$	
764 reflections	$(\Delta/\sigma)_{max} = 0.002$
72 parameters	$\Delta\rho_{max} = 0.19$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.29$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Refinement. Positions of amine H atoms were freely refined.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.2439 (2)	0.250000	0.29026 (13)	0.0223 (3)	
O2	0.8631 (2)	0.250000	0.75147 (13)	0.0242 (4)	
O3	0.6183 (2)	0.250000	0.58335 (14)	0.0335 (4)	
O4	0.4914 (3)	0.250000	0.78635 (15)	0.0339 (4)	
N1	0.1396 (3)	0.250000	0.16287 (16)	0.0240 (4)	
N2	−0.0807 (3)	0.250000	0.18624 (15)	0.0218 (4)	
N3	0.1429 (3)	0.250000	0.51217 (16)	0.0225 (4)	
H3A	0.296 (5)	0.250000	0.535 (2)	0.027*	
H3B	0.033 (4)	0.250000	0.571 (3)	0.027*	
N4	0.6555 (3)	0.250000	0.70870 (16)	0.0207 (4)	
C1	−0.1347 (3)	0.250000	0.31674 (18)	0.0220 (4)	
H1	−0.285332	0.250000	0.353916	0.026*	
C2	0.0778 (3)	0.250000	0.38510 (17)	0.0192 (4)	
C3	−0.2472 (4)	0.250000	0.0713 (2)	0.0325 (5)	
H3C	−0.164420	0.217972	−0.011556	0.049*	0.5
H3D	−0.322587	0.400144	0.064226	0.049*	0.5
H3E	−0.365475	0.131884	0.084774	0.049*	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0212 (7)	0.0245 (7)	0.0215 (7)	0.000	0.0047 (5)	0.000
O2	0.0196 (7)	0.0281 (7)	0.0248 (7)	0.000	−0.0023 (5)	0.000
O3	0.0252 (8)	0.0580 (10)	0.0173 (7)	0.000	−0.0012 (5)	0.000
O4	0.0252 (8)	0.0481 (9)	0.0289 (8)	0.000	0.0110 (6)	0.000
N1	0.0263 (8)	0.0267 (8)	0.0191 (7)	0.000	0.0033 (6)	0.000
N2	0.0248 (9)	0.0216 (7)	0.0190 (8)	0.000	0.0017 (6)	0.000
N3	0.0199 (8)	0.0277 (8)	0.0200 (8)	0.000	0.0025 (6)	0.000
N4	0.0213 (8)	0.0196 (7)	0.0213 (7)	0.000	0.0036 (6)	0.000
C1	0.0219 (9)	0.0241 (8)	0.0200 (9)	0.000	0.0042 (7)	0.000
C2	0.0207 (9)	0.0171 (8)	0.0200 (9)	0.000	0.0039 (7)	0.000
C3	0.0325 (11)	0.0434 (12)	0.0213 (9)	0.000	−0.0038 (8)	0.000

Geometric parameters (Å, º)

O1—C2	1.359 (2)	N3—H3B	0.87 (3)
O1—N1	1.389 (2)	C1—C2	1.383 (3)
O2—N4	1.257 (2)	C1—H1	0.9500
O3—N4	1.260 (2)	C3—H3C	0.9800
O4—N4	1.234 (2)	C3—H3D	0.9800
N1—N2	1.293 (2)	C3—H3E	0.9800
N2—C1	1.342 (2)	C3—H3C^i	0.980 (11)

N2—C3	1.473 (2)	C3—H3D^i	0.980 (16)
N3—C2	1.310 (2)	C3—H3E^i	0.98 (3)
N3—H3A	0.90 (3)		
C2—O1—N1	109.79 (14)	N3—C2—C1	134.65 (18)
N2—N1—O1	103.82 (14)	O1—C2—C1	106.58 (15)
N1—N2—C1	115.09 (16)	N2—C3—H3C	109.5
N1—N2—C3	118.75 (16)	N2—C3—H3D	109.5
C1—N2—C3	126.16 (17)	H3C—C3—H3D	109.5
C2—N3—H3A	120.0 (16)	N2—C3—H3E	109.5
C2—N3—H3B	117.0 (16)	H3C—C3—H3E	109.5
H3A—N3—H3B	123 (2)	H3D—C3—H3E	109.5
O4—N4—O2	121.45 (16)	N2—C3—H3C^i	109.5 (2)
O4—N4—O3	120.39 (16)	N2—C3—H3D^i	109.5 (3)
O2—N4—O3	118.16 (15)	H3C^i—C3—H3D^i	109.5
N2—C1—C2	104.71 (16)	N2—C3—H3E^i	109.5 (5)
N2—C1—H1	127.6	H3C^i—C3—H3E^i	109.5
C2—C1—H1	127.6	H3D^i—C3—H3E^i	109.5
N3—C2—O1	118.77 (17)		
C2—O1—N1—N2	0.000 (1)	N1—O1—C2—N3	180.000 (1)
O1—N1—N2—C1	0.000 (1)	N1—O1—C2—C1	0.000 (1)
O1—N1—N2—C3	180.000 (1)	N2—C1—C2—N3	180.000 (1)
N1—N2—C1—C2	0.000 (1)	N2—C1—C2—O1	0.000 (1)
C3—N2—C1—C2	180.000 (1)		

Symmetry code: (i) x, $-y+1/2$, z.

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O3	0.90 (3)	1.90 (3)	2.806 (2)	180 (2)
N3—H3B···O2^{ii}	0.87 (3)	2.06 (3)	2.905 (2)	162 (2)
N3—H3B···O3^{ii}	0.87 (3)	2.39 (3)	3.114 (2)	141 (2)
C1—H1···O3^{ii}	0.95	2.36	3.039 (2)	128
C3—H3C···O2^{iii}	0.98	2.37	3.260 (3)	150

Symmetry codes: (ii) $x-1$, y, z; (iii) $x-1$, y, $z-1$.

Compound 3
CCDC-2024996
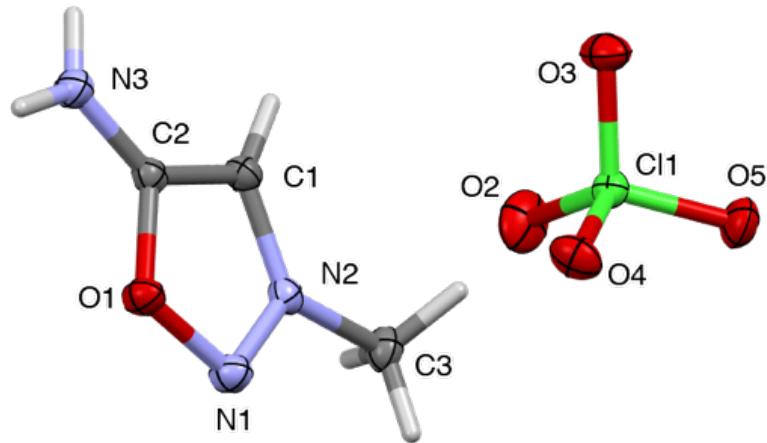
Fig. 2 Molecular unit 5-amino-3-methyl-1,2,3-oxadiazolium perchlorate (**3**). Ellipsoids are drawn at the 50% probability level.

Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$C_3H_6N_3O \cdot ClO_4$
M_r	199.56
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	150
a, b, c (Å)	19.5213 (6), 5.1844 (1), 14.8287 (5)
β (°)	104.6857 (11)
V (Å³)	1451.73 (7)
Z	8
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	0.52
Crystal size (mm)	0.55 × 0.17 × 0.13
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.677, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18329, 2673, 2415
R_{int}	0.031
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.071, 1.05
No. of reflections	2673
No. of parameters	117
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å⁻³)	0.49, −0.49

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

Table 2

Hydrogen-bond geometry (Å, º)

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C3—H3*A*⋯O2	0.98	2.61	3.0971 (13)	111
C3—H3*A*⋯O2[i]	0.98	2.55	3.4776 (14)	158
C3—H3*A*⋯O5[i]	0.98	2.66	3.2613 (14)	120
C3—H3*B*⋯O5[ii]	0.98	2.44	3.2182 (12)	136
N3—H3*D*⋯O3[iii]	0.809 (16)	2.160 (16)	2.9470 (12)	164.2 (14)
N3—H3*E*⋯O4[iv]	0.825 (16)	2.149 (16)	2.9610 (12)	168.3 (14)

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2; (ii) *x*, −*y*+1, *z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) *x*, −*y*, *z*+1/2.

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Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). J. Appl. Cryst., 37, 335–338.

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CSD: Groom, C. R. & Allen, F. H. (2014). Angew. Chem. Int. Ed., 53, 662–671.

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Figure 1

supporting information

Title

Computing details

Data collection: Apex3 v2019.1-0 (Bruker, 2019); cell refinement: *SAINT* V8.40A (Bruker, 2019); data reduction: *SAINT* V8.40A (Bruker, 2019); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

(G117E_MSI_CLO4_0m)

Crystal data

$C_3H_6N_3O \cdot ClO_4$	$F(000) = 816$
$M_r = 199.56$	$D_x = 1.826$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 19.5213$ (6) Å	Cell parameters from 9995 reflections
$b = 5.1844$ (1) Å	$\theta = 2.8–33.2°$
$c = 14.8287$ (5) Å	$\mu = 0.52$ mm^{-1}
$\beta = 104.6857$ (11)°	$T = 150$ K
$V = 1451.73$ (7) Å^3	Needle, colourless
$Z = 8$	$0.55 \times 0.17 \times 0.13$ mm

Data collection

Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)	Absorption correction: multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
Radiation source: fine focus sealed tube X-ray source	$T_{min} = 0.677$, $T_{max} = 0.747$
Triumph curved graphite crystal monochromator	18329 measured reflections
Detector resolution: 7.4074 pixels mm^{-1}	2673 independent reflections
ω and phi scans	2415 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.031$
	$\theta_{max} = 33.2°$, $\theta_{min} = 2.8°$
	$h = -30 \rightarrow 30$
	$k = -7 \rightarrow 6$
	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.025$	
$wR(F^2) = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 1.1237P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	
2673 reflections	$(\Delta/\sigma)_{max} = 0.001$
117 parameters	$\Delta\rho_{max} = 0.49$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.49$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL2018*/3 (Sheldrick 2018), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0056 (8)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Positions of N—H hydrogen atoms were freely refined.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}
C1	0.37449 (5)	0.33309 (18)	0.38989 (6)	0.01651 (16)
H1	0.408239	0.207815	0.419566	0.020*
C2	0.30172 (5)	0.32790 (18)	0.37751 (6)	0.01517 (16)
C3	0.45480 (5)	0.6624 (2)	0.34430 (7)	0.01991 (18)
H3A	0.482925	0.526370	0.325017	0.030*
H3B	0.480282	0.729143	0.405435	0.030*
H3C	0.446867	0.802625	0.298490	0.030*
N1	0.33018 (4)	0.69184 (17)	0.31466 (6)	0.01973 (16)
N2	0.38632 (4)	0.55619 (16)	0.35022 (5)	0.01531 (14)
N3	0.25701 (5)	0.16369 (17)	0.39905 (6)	0.01923 (16)
H3D	0.2152 (8)	0.196 (3)	0.3890 (10)	0.023*
H3E	0.2735 (8)	0.037 (3)	0.4310 (10)	0.023*
O1	0.27542 (4)	0.54576 (14)	0.33165 (5)	0.01915 (14)
O2	0.40655 (5)	0.27309 (19)	0.18218 (6)	0.0329 (2)
O3	0.38568 (4)	−0.13420 (15)	0.11009 (6)	0.02573 (17)
O4	0.32859 (4)	0.23462 (16)	0.03326 (5)	0.02487 (16)
O5	0.45103 (4)	0.17659 (17)	0.05259 (6)	0.02617 (17)
Cl1	0.39316 (2)	0.13921 (4)	0.09537 (2)	0.01512 (7)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0164 (4)	0.0160 (4)	0.0174 (4)	0.0024 (3)	0.0046 (3)	0.0010 (3)
C2	0.0165 (4)	0.0155 (4)	0.0135 (3)	0.0017 (3)	0.0037 (3)	−0.0007 (3)
C3	0.0175 (4)	0.0226 (5)	0.0212 (4)	−0.0032 (3)	0.0077 (3)	−0.0019 (3)
N1	0.0177 (3)	0.0187 (4)	0.0224 (4)	0.0010 (3)	0.0044 (3)	0.0039 (3)
N2	0.0161 (3)	0.0158 (3)	0.0143 (3)	0.0008 (2)	0.0043 (2)	−0.0016 (2)
N3	0.0173 (3)	0.0190 (4)	0.0223 (4)	0.0007 (3)	0.0067 (3)	0.0032 (3)
O1	0.0157 (3)	0.0185 (3)	0.0225 (3)	0.0018 (2)	0.0034 (2)	0.0045 (2)
O2	0.0398 (5)	0.0398 (5)	0.0190 (3)	−0.0105 (4)	0.0075 (3)	−0.0126 (3)
O3	0.0214 (3)	0.0171 (4)	0.0387 (4)	−0.0002 (3)	0.0077 (3)	0.0052 (3)
O4	0.0188 (3)	0.0232 (4)	0.0289 (4)	0.0051 (3)	−0.0010 (3)	0.0001 (3)
O5	0.0210 (3)	0.0318 (4)	0.0298 (4)	−0.0009 (3)	0.0138 (3)	0.0040 (3)
Cl1	0.01392 (10)	0.01654 (11)	0.01473 (10)	−0.00140 (6)	0.00335 (7)	−0.00132 (6)

Geometric parameters (Å, º)

C1—N2	1.3439 (12)	N1—N2	1.2964 (11)
C1—C2	1.3858 (12)	N1—O1	1.3843 (11)
C1—H1	0.9500	N3—H3D	0.809 (16)
C2—N3	1.3151 (12)	N3—H3E	0.825 (16)
C2—O1	1.3508 (11)	O2—Cl1	1.4271 (8)

C3—N2	1.4688 (12)	O3—Cl1	1.4472 (8)
C3—H3A	0.9800	O4—Cl1	1.4468 (7)
C3—H3B	0.9800	O5—Cl1	1.4422 (7)
C3—H3C	0.9800		
N2—C1—C2	104.06 (8)	N1—N2—C1	115.06 (8)
N2—C1—H1	128.0	N1—N2—C3	117.43 (8)
C2—C1—H1	128.0	C1—N2—C3	127.50 (8)
N3—C2—O1	118.20 (8)	C2—N3—H3D	121.4 (11)
N3—C2—C1	134.55 (9)	C2—N3—H3E	117.9 (10)
O1—C2—C1	107.24 (8)	H3D—N3—H3E	119.8 (14)
N2—C3—H3A	109.5	C2—O1—N1	109.67 (7)
N2—C3—H3B	109.5	O2—Cl1—O5	110.29 (5)
H3A—C3—H3B	109.5	O2—Cl1—O4	109.80 (5)
N2—C3—H3C	109.5	O5—Cl1—O4	109.10 (5)
H3A—C3—H3C	109.5	O2—Cl1—O3	110.04 (6)
H3B—C3—H3C	109.5	O5—Cl1—O3	108.55 (5)
N2—N1—O1	103.97 (7)	O4—Cl1—O3	109.02 (5)
N2—C1—C2—N3	179.16 (10)	C2—C1—N2—C3	179.08 (8)
N2—C1—C2—O1	0.11 (9)	N3—C2—O1—N1	−179.51 (8)
O1—N1—N2—C1	−0.28 (10)	C1—C2—O1—N1	−0.28 (10)
O1—N1—N2—C3	−179.35 (7)	N2—N1—O1—C2	0.33 (10)
C2—C1—N2—N1	0.11 (10)		

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C3—H3A⋯O2	0.98	2.61	3.0971 (13)	111
C3—H3A⋯O2[i]	0.98	2.55	3.4776 (14)	158
C3—H3A⋯O5[i]	0.98	2.66	3.2613 (14)	120
C3—H3B⋯O5[ii]	0.98	2.44	3.2182 (12)	136
N3—H3D⋯O3[iii]	0.809 (16)	2.160 (16)	2.9470 (12)	164.2 (14)
N3—H3E⋯O4[iv]	0.825 (16)	2.149 (16)	2.9610 (12)	168.3 (14)

Symmetry codes: (i) −x+1, y, −z+1/2; (ii) x, −y+1, z+1/2; (iii) −x+1/2, y+1/2, −z+1/2; (iv) x, −y, z+1/2.

Compound 4
CCDC-2024995
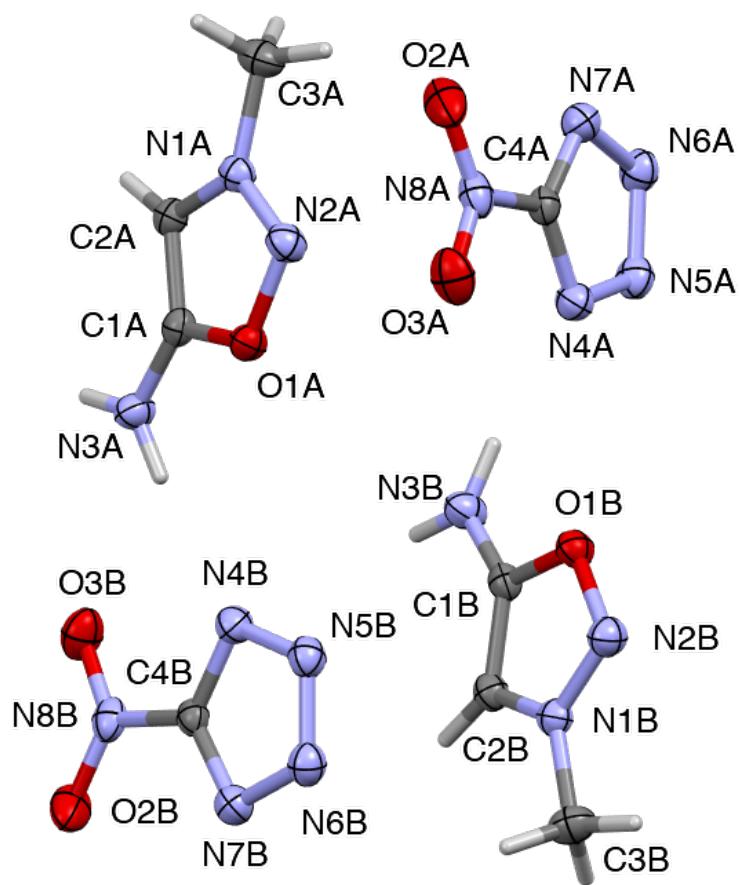
Fig. 3 Molecular units of 5-amino-3-methyl-1,2,3-oxadiazolium nitrotetrazolate (**4**). Ellipsoids are drawn at the 50% probability level.

Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$CN_5O_2 \cdot C_3H_6N_3O$
M_r	214.17
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	24.1038 (10), 5.0060 (2), 15.4562 (7)
β (°)	108.365 (3)
V (Å^3)	1770.01 (13)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.20
Crystal size (mm)	$0.14 \times 0.11 \times 0.07$
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.698, 0.753
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24473, 3112, 2737
R_{int}	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.077, 1.03
No. of reflections	3112
No. of parameters	290
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.17

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

Table 2

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3A—H3D⋯N4B	0.87 (1)	2.06 (1)	2.9186 (16)	173 (2)
N3A—H3E⋯N5A[i]	0.86 (1)	2.14 (1)	2.9498 (16)	157 (2)
C2A—H2A⋯N6A[i]	0.95	2.48	3.3273 (17)	148
C3A—H3A⋯N6A[ii]	0.98	2.70	3.3491 (17)	124
C3A—H3B⋯N7A[iii]	0.98	2.63	3.5140 (19)	149
C3A—H3C⋯O2A	0.98	2.61	3.5121 (19)	154
N3B—H3I⋯N5B	0.86 (1)	2.18 (1)	2.9759 (16)	154 (2)
N3B—H3J⋯N4A	0.87 (1)	2.06 (1)	2.9207 (16)	172 (2)
C2B—H2B⋯N5B	0.95	2.69	3.2722 (16)	120
C2B—H2B⋯N6B	0.95	2.45	3.3079 (17)	150
C3B—H3H⋯N7B[iv]	0.98	2.63	3.4890 (19)	146

Symmetry codes: (i) x, $-y+5/2$, $z-1/2$; (ii) x, $-y+3/2$, $z-1/2$; (iii) $-x$, $-y+2$, $-z+1$; (iv) $-x+1$, $y-1/2$, $-z+3/2$.

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publCIF: Westrip, S. P. (2010). J. Appl. Cryst., 43, 920–925.

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Spek, A. L. (2003). J. Appl. Cryst., 36, 7–13.

Figure 1

supporting information

Title

Computing details

Data collection: Apex3 v2019.1-0 (Bruker, 2019); cell refinement: *SAINT* V8.40A (Bruker, 2019); data reduction: *SAINT* V8.40A (Bruker, 2019); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

(G117_MSI_NT_0m)

Crystal data

$CN_5O_2 \cdot C_3H_6N_3O$	$F(000) = 880$
$M_r = 214.17$	$D_x = 1.607$ Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 24.1038\,(10)$ Å	Cell parameters from 9897 reflections
$b = 5.0060\,(2)$ Å	$\theta = 3.9\text{–}66.6°$
$c = 15.4562\,(7)$ Å	$\mu = 1.20$ mm^{-1}
$\beta = 108.365\,(3)°$	$T = 150$ K
$V = 1770.01\,(13)$ Å^3	Block, colourless
$Z = 8$	$0.14 \times 0.11 \times 0.07$ mm

Data collection

Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating pixel array detector (CPAD)	Absorption correction: multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
Radiation source: I-mu-S microsource X-ray tube	$T_{min} = 0.698$, $T_{max} = 0.753$
Laterally graded multilayer (Goebel) mirror monochromator	24473 measured reflections
Detector resolution: 7.4074 pixels mm^{-1}	3112 independent reflections
ω and phi scans	2737 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.038$
	$\theta_{max} = 66.7°$, $\theta_{min} = 3.9°$
	$h = -28 \rightarrow 26$
	$k = -5 \rightarrow 5$
	$l = -14 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.029$	
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	
3112 reflections	$(\Delta/\sigma)_{max} < 0.001$
290 parameters	$\Delta\rho_{max} = 0.20$ e Å^{-3}
6 restraints	$\Delta\rho_{min} = -0.17$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL2018*/3 (Sheldrick 2018), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.00137 (16)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Amine H atom positions were refined and N—H distances were restrained to be similar to each other.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}
O1A	0.18972 (4)	0.90404 (18)	0.47750 (6)	0.0235 (2)
O2A	0.07589 (5)	0.2800 (2)	0.55620 (7)	0.0406 (3)
O3A	0.17044 (5)	0.2789 (2)	0.61305 (7)	0.0380 (3)
N1A	0.09782 (5)	0.9056 (2)	0.41950 (7)	0.0217 (2)
N2A	0.13915 (5)	0.7713 (2)	0.47702 (7)	0.0254 (3)
N3A	0.21741 (5)	1.2718 (2)	0.41215 (8)	0.0267 (3)
H3D	0.2523 (6)	1.267 (4)	0.4511 (10)	0.036 (4)*
H3E	0.2061 (7)	1.395 (3)	0.3716 (10)	0.032 (4)*
N4A	0.16678 (5)	0.6988 (2)	0.72092 (7)	0.0248 (2)
N5A	0.14563 (5)	0.8862 (2)	0.76345 (7)	0.0262 (3)
N6A	0.08781 (5)	0.8762 (2)	0.73533 (7)	0.0274 (3)
N7A	0.06953 (5)	0.6814 (2)	0.67330 (7)	0.0269 (3)
N8A	0.12221 (5)	0.3637 (2)	0.60845 (7)	0.0269 (3)
C1A	0.17573 (5)	1.1165 (3)	0.42069 (8)	0.0204 (3)
C2A	0.11573 (5)	1.1167 (3)	0.38192 (8)	0.0213 (3)
H2A	0.092399	1.238730	0.338471	0.026*
C3A	0.03717 (6)	0.8194 (3)	0.40363 (10)	0.0307 (3)
H3A	0.021927	0.739205	0.342880	0.046*
H3B	0.013184	0.974081	0.407621	0.046*
H3C	0.035949	0.687352	0.449809	0.046*
C4A	0.11919 (5)	0.5820 (3)	0.66772 (8)	0.0211 (3)
O1B	0.31253 (4)	0.38489 (18)	0.79026 (6)	0.0241 (2)
O2B	0.41986 (5)	1.7242 (2)	0.48258 (6)	0.0381 (3)
O3B	0.32534 (5)	1.6988 (2)	0.44037 (6)	0.0344 (2)
N1B	0.40444 (5)	0.4056 (2)	0.82399 (7)	0.0218 (2)
N2B	0.36412 (5)	0.2615 (2)	0.84034 (7)	0.0255 (3)
N3B	0.28172 (5)	0.7468 (2)	0.69660 (8)	0.0278 (3)
H3I	0.2915 (7)	0.873 (3)	0.6667 (10)	0.032 (4)*
H3J	0.2465 (6)	0.722 (4)	0.6989 (11)	0.039 (5)*
N4B	0.33125 (5)	1.2795 (2)	0.55329 (7)	0.0249 (3)
N5B	0.35342 (5)	1.0976 (2)	0.61825 (7)	0.0256 (3)
N6B	0.41108 (5)	1.1218 (2)	0.64990 (7)	0.0265 (3)
N7B	0.42816 (5)	1.3210 (2)	0.60622 (7)	0.0263 (3)
N8B	0.37401 (5)	1.6265 (2)	0.48632 (7)	0.0251 (3)
C1B	0.32484 (5)	0.6008 (3)	0.74706 (8)	0.0208 (3)
C2B	0.38483 (5)	0.6140 (3)	0.76830 (8)	0.0214 (3)
H2B	0.407162	0.741697	0.748063	0.026*
C3B	0.46547 (6)	0.3283 (3)	0.86818 (10)	0.0318 (3)
H3F	0.481553	0.252781	0.822650	0.048*
H3G	0.467440	0.194556	0.915358	0.048*
H3H	0.488231	0.485902	0.896088	0.048*
C4B	0.37816 (5)	1.4085 (3)	0.54896 (8)	0.0202 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1A	0.0220 (5)	0.0234 (5)	0.0244 (4)	0.0014 (4)	0.0065 (3)	0.0039 (4)
O2A	0.0491 (7)	0.0433 (7)	0.0346 (5)	−0.0234 (5)	0.0205 (5)	−0.0175 (5)
O3A	0.0487 (7)	0.0325 (6)	0.0398 (6)	0.0099 (5)	0.0240 (5)	0.0000 (4)
N1A	0.0220 (5)	0.0215 (6)	0.0224 (5)	0.0002 (4)	0.0083 (4)	−0.0017 (4)
N2A	0.0252 (6)	0.0243 (6)	0.0283 (5)	−0.0007 (4)	0.0104 (5)	0.0035 (4)
N3A	0.0215 (6)	0.0294 (7)	0.0262 (6)	−0.0020 (5)	0.0034 (5)	0.0059 (5)
N4A	0.0241 (6)	0.0262 (6)	0.0248 (5)	−0.0015 (5)	0.0085 (4)	−0.0014 (5)
N5A	0.0306 (6)	0.0246 (6)	0.0238 (5)	−0.0026 (5)	0.0090 (4)	−0.0025 (4)
N6A	0.0302 (6)	0.0275 (6)	0.0248 (5)	0.0032 (5)	0.0090 (5)	−0.0016 (5)
N7A	0.0247 (6)	0.0304 (6)	0.0247 (5)	−0.0002 (5)	0.0066 (4)	−0.0013 (5)
N8A	0.0378 (7)	0.0222 (6)	0.0257 (5)	−0.0048 (5)	0.0170 (5)	−0.0004 (4)
C1A	0.0238 (6)	0.0198 (6)	0.0177 (5)	0.0021 (5)	0.0066 (5)	0.0001 (5)
C2A	0.0229 (6)	0.0205 (7)	0.0200 (6)	0.0007 (5)	0.0060 (5)	0.0002 (5)
C3A	0.0228 (7)	0.0323 (8)	0.0385 (7)	−0.0039 (6)	0.0119 (6)	−0.0022 (6)
C4A	0.0252 (6)	0.0214 (6)	0.0185 (5)	−0.0016 (5)	0.0093 (5)	0.0007 (5)
O1B	0.0231 (5)	0.0239 (5)	0.0260 (4)	−0.0016 (4)	0.0088 (4)	0.0033 (4)
O2B	0.0444 (6)	0.0405 (6)	0.0283 (5)	−0.0212 (5)	0.0102 (4)	0.0025 (4)
O3B	0.0410 (6)	0.0321 (6)	0.0279 (5)	0.0090 (5)	0.0075 (4)	0.0061 (4)
N1B	0.0224 (5)	0.0217 (6)	0.0213 (5)	−0.0001 (4)	0.0071 (4)	−0.0014 (4)
N2B	0.0251 (6)	0.0251 (6)	0.0254 (5)	0.0002 (5)	0.0066 (4)	0.0037 (4)
N3B	0.0225 (6)	0.0288 (7)	0.0331 (6)	0.0016 (5)	0.0102 (5)	0.0083 (5)
N4B	0.0247 (6)	0.0263 (6)	0.0232 (5)	−0.0034 (5)	0.0068 (4)	0.0017 (4)
N5B	0.0288 (6)	0.0249 (6)	0.0243 (5)	−0.0022 (5)	0.0099 (4)	0.0018 (4)
N6B	0.0298 (6)	0.0254 (6)	0.0245 (5)	0.0023 (5)	0.0090 (5)	0.0026 (4)
N7B	0.0249 (6)	0.0289 (6)	0.0257 (5)	−0.0007 (5)	0.0090 (4)	0.0014 (5)
N8B	0.0343 (6)	0.0222 (6)	0.0185 (5)	−0.0042 (5)	0.0077 (5)	−0.0032 (4)
C1B	0.0244 (6)	0.0203 (7)	0.0200 (6)	−0.0018 (5)	0.0102 (5)	−0.0008 (5)
C2B	0.0234 (6)	0.0200 (7)	0.0219 (6)	−0.0009 (5)	0.0089 (5)	−0.0003 (5)
C3B	0.0237 (7)	0.0342 (8)	0.0338 (7)	0.0031 (6)	0.0040 (6)	0.0004 (6)
C4B	0.0235 (6)	0.0209 (6)	0.0169 (5)	−0.0018 (5)	0.0074 (5)	−0.0023 (5)

Geometric parameters (Å, º)

O1A—C1A	1.3525 (15)	O1B—C1B	1.3516 (15)
O1A—N2A	1.3863 (14)	O1B—N2B	1.3856 (14)
O2A—N8A	1.2272 (16)	O2B—N8B	1.2263 (15)
O3A—N8A	1.2185 (16)	O3B—N8B	1.2192 (15)
N1A—N2A	1.2949 (16)	N1B—N2B	1.2973 (16)
N1A—C2A	1.3411 (17)	N1B—C2B	1.3403 (17)
N1A—C3A	1.4687 (16)	N1B—C3B	1.4653 (17)
N3A—C1A	1.3095 (18)	N3B—C1B	1.3082 (18)
N3A—H3D	0.868 (14)	N3B—H3I	0.858 (13)
N3A—H3E	0.861 (13)	N3B—H3J	0.869 (14)
N4A—C4A	1.3189 (17)	N4B—C4B	1.3217 (17)
N4A—N5A	1.3352 (16)	N4B—N5B	1.3360 (16)
N5A—N6A	1.3236 (16)	N5B—N6B	1.3256 (16)
N6A—N7A	1.3408 (17)	N6B—N7B	1.3396 (16)
N7A—C4A	1.3240 (17)	N7B—C4B	1.3250 (17)
N8A—C4A	1.4422 (17)	N8B—C4B	1.4416 (17)

C1A—C2A	1.3800 (18)	C1B—C2B	1.3799 (18)
C2A—H2A	0.9500	C2B—H2B	0.9500
C3A—H3A	0.9800	C3B—H3F	0.9800
C3A—H3B	0.9800	C3B—H3G	0.9800
C3A—H3C	0.9800	C3B—H3H	0.9800
C1A—O1A—N2A	109.54 (9)	C1B—O1B—N2B	109.54 (9)
N2A—N1A—C2A	115.05 (10)	N2B—N1B—C2B	115.06 (11)
N2A—N1A—C3A	118.17 (11)	N2B—N1B—C3B	117.79 (11)
C2A—N1A—C3A	126.76 (11)	C2B—N1B—C3B	127.14 (11)
N1A—N2A—O1A	103.87 (9)	N1B—N2B—O1B	103.83 (9)
C1A—N3A—H3D	121.4 (11)	C1B—N3B—H3I	115.5 (11)
C1A—N3A—H3E	115.0 (11)	C1B—N3B—H3J	119.8 (12)
H3D—N3A—H3E	122.7 (16)	H3I—N3B—H3J	124.4 (16)
C4A—N4A—N5A	103.09 (10)	C4B—N4B—N5B	103.01 (10)
N6A—N5A—N4A	109.73 (10)	N6B—N5B—N4B	109.84 (10)
N5A—N6A—N7A	109.71 (10)	N5B—N6B—N7B	109.59 (10)
C4A—N7A—N6A	102.68 (11)	C4B—N7B—N6B	102.90 (10)
O3A—N8A—O2A	124.94 (12)	O3B—N8B—O2B	124.76 (12)
O3A—N8A—C4A	117.72 (12)	O3B—N8B—C4B	117.79 (11)
O2A—N8A—C4A	117.34 (11)	O2B—N8B—C4B	117.45 (11)
N3A—C1A—O1A	119.34 (11)	N3B—C1B—O1B	118.97 (11)
N3A—C1A—C2A	133.48 (12)	N3B—C1B—C2B	133.73 (12)
O1A—C1A—C2A	107.17 (11)	O1B—C1B—C2B	107.29 (11)
N1A—C2A—C1A	104.34 (11)	N1B—C2B—C1B	104.28 (11)
N1A—C2A—H2A	127.8	N1B—C2B—H2B	127.9
C1A—C2A—H2A	127.8	C1B—C2B—H2B	127.9
N1A—C3A—H3A	109.5	N1B—C3B—H3F	109.5
N1A—C3A—H3B	109.5	N1B—C3B—H3G	109.5
H3A—C3A—H3B	109.5	H3F—C3B—H3G	109.5
N1A—C3A—H3C	109.5	N1B—C3B—H3H	109.5
H3A—C3A—H3C	109.5	H3F—C3B—H3H	109.5
H3B—C3A—H3C	109.5	H3G—C3B—H3H	109.5
N4A—C4A—N7A	114.79 (11)	N4B—C4B—N7B	114.67 (11)
N4A—C4A—N8A	121.59 (11)	N4B—C4B—N8B	121.63 (11)
N7A—C4A—N8A	123.61 (12)	N7B—C4B—N8B	123.70 (11)
C2A—N1A—N2A—O1A	−0.51 (13)	C2B—N1B—N2B—O1B	0.37 (13)
C3A—N1A—N2A—O1A	−178.95 (10)	C3B—N1B—N2B—O1B	179.56 (10)
C1A—O1A—N2A—N1A	1.10 (12)	C1B—O1B—N2B—N1B	−0.84 (12)
C4A—N4A—N5A—N6A	0.01 (13)	C4B—N4B—N5B—N6B	−0.05 (13)
N4A—N5A—N6A—N7A	−0.07 (14)	N4B—N5B—N6B—N7B	−0.04 (14)
N5A—N6A—N7A—C4A	0.10 (13)	N5B—N6B—N7B—C4B	0.10 (13)
N2A—O1A—C1A—N3A	179.05 (11)	N2B—O1B—C1B—N3B	−179.34 (11)
N2A—O1A—C1A—C2A	−1.28 (12)	N2B—O1B—C1B—C2B	0.99 (13)
N2A—N1A—C2A—C1A	−0.25 (14)	N2B—N1B—C2B—C1B	0.21 (14)
C3A—N1A—C2A—C1A	178.04 (11)	C3B—N1B—C2B—C1B	−178.88 (12)
N3A—C1A—C2A—N1A	−179.47 (13)	N3B—C1B—C2B—N1B	179.67 (14)
O1A—C1A—C2A—N1A	0.92 (13)	O1B—C1B—C2B—N1B	−0.73 (13)
N5A—N4A—C4A—N7A	0.06 (14)	N5B—N4B—C4B—N7B	0.12 (14)
N5A—N4A—C4A—N8A	179.87 (11)	N5B—N4B—C4B—N8B	−179.84 (10)
N6A—N7A—C4A—N4A	−0.10 (14)	N6B—N7B—C4B—N4B	−0.14 (14)

N6A—N7A—C4A—N8A	−179.91 (11)	N6B—N7B—C4B—N8B		179.82 (11)
O3A—N8A—C4A—N4A	4.43 (17)	O3B—N8B—C4B—N4B		3.85 (17)
O2A—N8A—C4A—N4A	−174.56 (12)	O2B—N8B—C4B—N4B		−175.48 (11)
O3A—N8A—C4A—N7A	−175.77 (12)	O3B—N8B—C4B—N7B		−176.11 (11)
O2A—N8A—C4A—N7A	5.24 (18)	O2B—N8B—C4B—N7B		4.56 (18)

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3A—H3$D\cdots$N4B	0.87 (1)	2.06 (1)	2.9186 (16)	173 (2)
N3A—H3$E\cdots$N5A^{i}	0.86 (1)	2.14 (1)	2.9498 (16)	157 (2)
C2A—H2$A\cdots$N6A^{i}	0.95	2.48	3.3273 (17)	148
C3A—H3$A\cdots$N6A^{ii}	0.98	2.70	3.3491 (17)	124
C3A—H3$B\cdots$N7A^{iii}	0.98	2.63	3.5140 (19)	149
C3A—H3$C\cdots$O2A	0.98	2.61	3.5121 (19)	154
N3B—H3$I\cdots$N5B	0.86 (1)	2.18 (1)	2.9759 (16)	154 (2)
N3B—H3$J\cdots$N4A	0.87 (1)	2.06 (1)	2.9207 (16)	172 (2)
C2B—H2$B\cdots$N5B	0.95	2.69	3.2722 (16)	120
C2B—H2$B\cdots$N6B	0.95	2.45	3.3079 (17)	150
C3B—H3$H\cdots$N7B^{iv}	0.98	2.63	3.4890 (19)	146

Symmetry codes: (i) x, $-y+5/2$, $z-1/2$; (ii) x, $-y+3/2$, $z-1/2$; (iii) $-x$, $-y+2$, $-z+1$; (iv) $-x+1$, $y-1/2$, $-z+3/2$.

**Compound 5**
CCDC-2024997
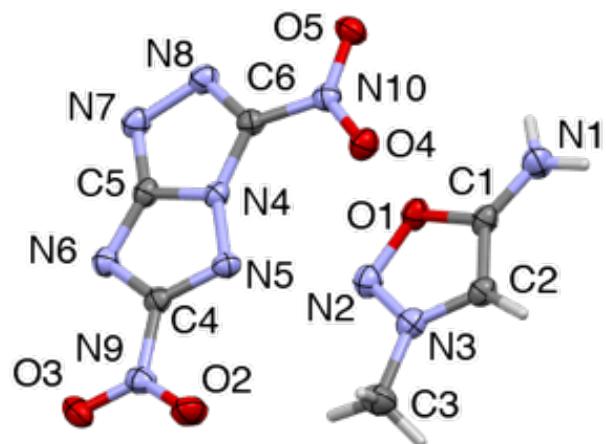
Fig. 4 Molecular unit of 5-amino-3-methyl-1,2,3-oxadiazolium DNTT (**5**). Ellipsoids are drawn at the 50% probability level.

Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$C_3N_7O_4 \cdot C_3H_6N_3O$
M_r	298.21
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	150
a, b, c (Å)	7.2060 (4), 9.3911 (5), 9.4448 (5)
α, β, γ (°)	71.6516 (19), 85.772 (2), 71.196 (2)
V (Å^3)	574.01 (5)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.15
Crystal size (mm)	$0.24 \times 0.20 \times 0.13$
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.676, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19787, 4208, 2910
R_{int}	0.053
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.043, 0.107, 1.02
No. of reflections	4208
No. of parameters	243
No. of restraints	37
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.41, −0.26

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

Table 2

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C2—H2⋯N6[i]	0.95	2.42	3.2951 (17)	154
C2—H2⋯N7B[i]	0.95	2.58	3.111 (15)	116
C2—H2⋯N8B[i]	0.95	1.95	2.789 (18)	147
C3—H3A⋯O4[ii]	0.98	2.60	3.4557 (18)	146
C3—H3C⋯O2B[iii]	0.98	2.05	2.88 (2)	140
C3—H3C⋯O3B[iii]	0.98	2.45	3.38 (2)	159
C3—H3C⋯N9B[iii]	0.98	2.59	3.544 (16)	165
N1—H1A⋯O5[iv]	0.854 (19)	2.342 (19)	3.1010 (17)	148.3 (15)
N1—H1A⋯N8[iv]	0.854 (19)	2.330 (18)	3.0269 (17)	139.1 (15)
N1—H1A⋯O3B[iv]	0.854 (19)	2.58 (3)	3.29 (2)	141.3 (16)
N1—H1A⋯N6B[iv]	0.854 (19)	2.56 (3)	3.342 (17)	152.5 (16)
N1—H1B⋯N7[i]	0.898 (19)	2.02 (2)	2.9131 (16)	173.9 (17)
N1—H1B⋯N7B[i]	0.898 (19)	1.97 (2)	2.748 (15)	144.0 (17)

Symmetry codes: (i) x, y−1, z; (ii) −x+1, −y+1, −z+1; (iii) x+1, y, z; (iv) −x, −y+1, −z+2.

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Figure 1

supporting information

Title

Computing details

Data collection: Apex3 v2019.1-0 (Bruker, 2019); cell refinement: *SAINT* V8.40A (Bruker, 2019); data reduction: *SAINT* V8.40A (Bruker, 2019); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

(G117_MSI_DNTT_0m)

Crystal data

$C_3N_7O_4 \cdot C_3H_6N_3O$
$M_r = 298.21$
Triclinic, $P\bar{1}$
$a = 7.2060 (4)$ Å
$b = 9.3911 (5)$ Å
$c = 9.4448 (5)$ Å
$\alpha = 71.6516 (19)°$
$\beta = 85.772 (2)°$
$\gamma = 71.196 (2)°$
$V = 574.01 (5)$ Å^3

$Z = 2$
$F(000) = 304$
$D_x = 1.725$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6327 reflections
$\theta = 2.8–33.2°$
$\mu = 0.15$ mm^{-1}
$T = 150$ K
Block, colourless
$0.24 \times 0.20 \times 0.13$ mm

Data collection

Bruker AXS D8 Quest
　diffractometer with PhotonII charge-integrating pixel
　array detector (CPAD)
Radiation source: fine focus sealed tube X-ray source
Triumph curved graphite crystal monochromator
Detector resolution: 7.4074 pixels mm^{-1}
ω and phi scans

Absorption correction: multi-scan
　SADABS 2016/2: Krause, L., Herbst-Irmer, R.,
　Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015)
　3-10
$T_{min} = 0.676$, $T_{max} = 0.747$
19787 measured reflections
4208 independent reflections
2910 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 33.2°$, $\theta_{min} = 2.3°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.107$
$S = 1.02$
4208 reflections
243 parameters
37 restraints
Primary atom site location: structure-invariant direct
　methods
Secondary atom site location: difference Fourier map

Hydrogen site location: mixed
H atoms treated by a mixture of independent and
　constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.1194P]$
　where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXL2018*/3 (Sheldrick
　2018), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.024 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. The anion exhibits minor disorder in place over two alternative orientations. The two disordered moieties were restrained to have similar geometries. U^{ij} components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar. Equivalent atoms in the major and minor moiuety were constrained to have identical ADPs. Subject to these conditions the occupancy ratio refined to 0.9467 (10) to 0.0533 (10).

Amine H atoms were freely refined.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.39717 (18)	0.23491 (14)	0.90203 (13)	0.0238 (2)	
C2	0.53967 (18)	0.20947 (14)	0.79838 (13)	0.0241 (2)	
H2	0.563608	0.136476	0.743511	0.029*	
C3	0.8024 (2)	0.33334 (19)	0.69825 (17)	0.0373 (3)	
H3A	0.754580	0.391215	0.594983	0.056*	
H3B	0.896565	0.229858	0.702665	0.056*	
H3C	0.866637	0.393606	0.733924	0.056*	
N1	0.25846 (19)	0.17317 (15)	0.95677 (14)	0.0315 (3)	
H1A	0.181 (3)	0.202 (2)	1.022 (2)	0.040 (5)*	
H1B	0.239 (3)	0.098 (2)	0.925 (2)	0.043 (5)*	
N2	0.57393 (17)	0.39806 (13)	0.88094 (12)	0.0282 (2)	
N3	0.63640 (16)	0.31137 (12)	0.79297 (11)	0.0255 (2)	
O1	0.41906 (14)	0.34912 (10)	0.95179 (10)	0.0264 (2)	
C4	0.57851 (19)	0.81021 (15)	0.61133 (14)	0.0216 (2)	0.9467 (10)
C5	0.36479 (19)	0.87773 (14)	0.75358 (13)	0.0221 (2)	0.9467 (10)
C6	0.16908 (18)	0.74095 (16)	0.77790 (14)	0.0215 (2)	0.9467 (10)
O2	0.78883 (16)	0.71131 (13)	0.44546 (13)	0.0362 (2)	0.9467 (10)
O3	0.8487 (2)	0.8872 (2)	0.5241 (2)	0.0313 (3)	0.9467 (10)
O4	0.15991 (15)	0.54893 (12)	0.68523 (11)	0.0293 (2)	0.9467 (10)
O5	−0.06586 (17)	0.62040 (16)	0.83931 (15)	0.0302 (3)	0.9467 (10)
N4	0.33355 (16)	0.76358 (14)	0.70752 (13)	0.0200 (2)	0.9467 (10)
N5	0.47352 (15)	0.71643 (12)	0.61130 (11)	0.0218 (2)	0.9467 (10)
N6	0.52634 (17)	0.91041 (14)	0.69238 (13)	0.0232 (2)	0.9467 (10)
N7	0.22537 (17)	0.92463 (13)	0.84734 (12)	0.0261 (2)	0.9467 (10)
N8	0.10328 (17)	0.83587 (14)	0.86069 (13)	0.0254 (2)	0.9467 (10)
N9	0.75137 (17)	0.80184 (14)	0.52034 (13)	0.0251 (2)	0.9467 (10)
N10	0.08232 (17)	0.62977 (14)	0.76714 (12)	0.0233 (2)	0.9467 (10)
C4B	0.164 (3)	0.687 (2)	0.746 (2)	0.0216 (2)	0.0533 (10)
C5B	0.277 (3)	0.848 (2)	0.785 (2)	0.0221 (2)	0.0533 (10)
C6B	0.539 (3)	0.844 (3)	0.659 (2)	0.0215 (2)	0.0533 (10)
O2B	0.087 (3)	0.494 (2)	0.679 (2)	0.0362 (2)	0.0533 (10)
O3B	−0.101 (3)	0.598 (4)	0.829 (3)	0.0313 (3)	0.0533 (10)
O4B	0.692 (3)	0.7029 (19)	0.504 (2)	0.0293 (2)	0.0533 (10)
O5B	0.814 (5)	0.872 (5)	0.537 (5)	0.0302 (3)	0.0533 (10)
N4B	0.392 (3)	0.775 (3)	0.691 (3)	0.0200 (2)	0.0533 (10)
N5B	0.324 (2)	0.6682 (19)	0.6599 (19)	0.0218 (2)	0.0533 (10)
N6B	0.130 (3)	0.787 (2)	0.825 (2)	0.0232 (2)	0.0533 (10)
N7B	0.353 (3)	0.950 (2)	0.810 (2)	0.0261 (2)	0.0533 (10)
N8B	0.518 (3)	0.949 (3)	0.726 (2)	0.0254 (2)	0.0533 (10)

N9B	0.046 (3)	0.586 (2)	0.753 (2)	0.0251 (2)	0.0533 (10)
N10B	0.690 (3)	0.802 (2)	0.566 (2)	0.0233 (2)	0.0533 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0292 (6)	0.0210 (5)	0.0210 (5)	−0.0058 (4)	−0.0002 (4)	−0.0083 (4)
C2	0.0270 (6)	0.0246 (5)	0.0217 (5)	−0.0069 (4)	0.0008 (4)	−0.0097 (4)
C3	0.0333 (7)	0.0414 (8)	0.0406 (8)	−0.0158 (6)	0.0115 (6)	−0.0154 (6)
N1	0.0372 (6)	0.0324 (6)	0.0315 (6)	−0.0146 (5)	0.0113 (5)	−0.0176 (5)
N2	0.0328 (6)	0.0261 (5)	0.0275 (5)	−0.0100 (4)	0.0016 (4)	−0.0101 (4)
N3	0.0277 (5)	0.0248 (5)	0.0230 (5)	−0.0061 (4)	−0.0006 (4)	−0.0080 (4)
O1	0.0334 (5)	0.0236 (4)	0.0243 (4)	−0.0089 (3)	0.0028 (3)	−0.0110 (3)
C4	0.0211 (6)	0.0207 (5)	0.0210 (5)	−0.0047 (4)	−0.0006 (4)	−0.0054 (4)
C5	0.0258 (6)	0.0201 (5)	0.0206 (5)	−0.0060 (5)	−0.0013 (4)	−0.0075 (4)
C6	0.0216 (6)	0.0224 (6)	0.0205 (5)	−0.0066 (5)	0.0008 (4)	−0.0070 (5)
O2	0.0311 (5)	0.0428 (6)	0.0412 (6)	−0.0121 (5)	0.0115 (4)	−0.0235 (5)
O3	0.0261 (7)	0.0329 (6)	0.0342 (6)	−0.0150 (5)	−0.0015 (5)	−0.0029 (5)
O4	0.0320 (5)	0.0282 (5)	0.0310 (5)	−0.0086 (4)	0.0028 (4)	−0.0150 (4)
O5	0.0260 (6)	0.0345 (6)	0.0333 (5)	−0.0141 (4)	0.0060 (5)	−0.0112 (4)
N4	0.0209 (6)	0.0194 (5)	0.0199 (5)	−0.0053 (4)	0.0002 (4)	−0.0074 (4)
N5	0.0208 (5)	0.0230 (5)	0.0217 (5)	−0.0055 (4)	0.0026 (4)	−0.0090 (4)
N6	0.0244 (5)	0.0228 (5)	0.0235 (5)	−0.0079 (4)	−0.0004 (4)	−0.0079 (4)
N7	0.0298 (6)	0.0257 (5)	0.0251 (5)	−0.0079 (4)	0.0028 (4)	−0.0124 (4)
N8	0.0268 (6)	0.0262 (5)	0.0241 (5)	−0.0074 (4)	0.0029 (4)	−0.0104 (4)
N9	0.0213 (5)	0.0264 (5)	0.0246 (5)	−0.0062 (4)	−0.0007 (4)	−0.0047 (4)
N10	0.0224 (5)	0.0236 (5)	0.0225 (5)	−0.0060 (4)	−0.0001 (4)	−0.0063 (4)
C4B	0.0211 (6)	0.0207 (5)	0.0210 (5)	−0.0047 (4)	−0.0006 (4)	−0.0054 (4)
C5B	0.0258 (6)	0.0201 (5)	0.0206 (5)	−0.0060 (5)	−0.0013 (4)	−0.0075 (4)
C6B	0.0216 (6)	0.0224 (6)	0.0205 (5)	−0.0066 (5)	0.0008 (4)	−0.0070 (5)
O2B	0.0311 (5)	0.0428 (6)	0.0412 (6)	−0.0121 (5)	0.0115 (4)	−0.0235 (5)
O3B	0.0261 (7)	0.0329 (6)	0.0342 (6)	−0.0150 (5)	−0.0015 (5)	−0.0029 (5)
O4B	0.0320 (5)	0.0282 (5)	0.0310 (5)	−0.0086 (4)	0.0028 (4)	−0.0150 (4)
O5B	0.0260 (6)	0.0345 (6)	0.0333 (5)	−0.0141 (4)	0.0060 (5)	−0.0112 (4)
N4B	0.0209 (6)	0.0194 (5)	0.0199 (5)	−0.0053 (4)	0.0002 (4)	−0.0074 (4)
N5B	0.0208 (5)	0.0230 (5)	0.0217 (5)	−0.0055 (4)	0.0026 (4)	−0.0090 (4)
N6B	0.0244 (5)	0.0228 (5)	0.0235 (5)	−0.0079 (4)	−0.0004 (4)	−0.0079 (4)
N7B	0.0298 (6)	0.0257 (5)	0.0251 (5)	−0.0079 (4)	0.0028 (4)	−0.0124 (4)
N8B	0.0268 (6)	0.0262 (5)	0.0241 (5)	−0.0074 (4)	0.0029 (4)	−0.0104 (4)
N9B	0.0213 (5)	0.0264 (5)	0.0246 (5)	−0.0062 (4)	−0.0007 (4)	−0.0047 (4)
N10B	0.0224 (5)	0.0236 (5)	0.0225 (5)	−0.0060 (4)	−0.0001 (4)	−0.0063 (4)

Geometric parameters (Å, º)

C1—N1	1.3081 (18)	O2—N9	1.2241 (15)
C1—O1	1.3541 (14)	O3—N9	1.2326 (17)
C1—C2	1.3823 (17)	O4—N10	1.2328 (14)
C2—N3	1.3410 (17)	O5—N10	1.2362 (15)
C2—H2	0.9500	N4—N5	1.3674 (14)
C3—N3	1.4691 (17)	N7—N8	1.3693 (17)
C3—H3A	0.9800	C4B—N6B	1.330 (16)
C3—H3B	0.9800	C4B—N5B	1.355 (16)

C3—H3C	0.9800	C4B—N9B	1.450 (15)
N1—H1A	0.854 (19)	C5B—N7B	1.335 (15)
N1—H1B	0.898 (19)	C5B—N6B	1.336 (15)
N2—N3	1.3000 (14)	C5B—N4B	1.364 (16)
N2—O1	1.3897 (15)	C6B—N8B	1.301 (16)
C4—N5	1.3334 (16)	C6B—N4B	1.378 (15)
C4—N6	1.3401 (16)	C6B—N10B	1.381 (15)
C4—N9	1.4552 (17)	O2B—N9B	1.226 (16)
C5—N6	1.3427 (18)	O3B—N9B	1.234 (17)
C5—N7	1.3478 (16)	O4B—N10B	1.236 (16)
C5—N4	1.3612 (16)	O5B—N10B	1.240 (17)
C6—N8	1.3201 (16)	N4B—N5B	1.363 (15)
C6—N4	1.3597 (16)	N7B—N8B	1.377 (16)
C6—N10	1.4102 (18)		
N1—C1—O1	118.73 (11)	C4—N5—N4	97.84 (10)
N1—C1—C2	134.08 (12)	C4—N6—C5	99.31 (11)
O1—C1—C2	107.19 (11)	C5—N7—N8	105.45 (10)
N3—C2—C1	104.21 (10)	C6—N8—N7	108.64 (11)
N3—C2—H2	127.9	O2—N9—O3	124.89 (13)
C1—C2—H2	127.9	O2—N9—C4	117.70 (12)
N3—C3—H3A	109.5	O3—N9—C4	117.41 (13)
N3—C3—H3B	109.5	O4—N10—O5	124.57 (12)
H3A—C3—H3B	109.5	O4—N10—C6	117.27 (11)
N3—C3—H3C	109.5	O5—N10—C6	118.16 (11)
H3A—C3—H3C	109.5	N6B—C4B—N5B	120.0 (14)
H3B—C3—H3C	109.5	N6B—C4B—N9B	123.7 (14)
C1—N1—H1A	122.6 (12)	N5B—C4B—N9B	116.2 (14)
C1—N1—H1B	120.9 (12)	N7B—C5B—N6B	141.9 (16)
H1A—N1—H1B	116.5 (16)	N7B—C5B—N4B	109.6 (13)
N3—N2—O1	103.41 (10)	N6B—C5B—N4B	108.4 (13)
N2—N3—C2	115.42 (11)	N8B—C6B—N4B	112.3 (14)
N2—N3—C3	118.19 (11)	N8B—C6B—N10B	125.4 (15)
C2—N3—C3	126.39 (11)	N4B—C6B—N10B	122.3 (15)
C1—O1—N2	109.77 (9)	N5B—N4B—C5B	113.3 (12)
N5—C4—N6	121.08 (12)	N5B—N4B—C6B	143.1 (14)
N5—C4—N9	118.34 (11)	C5B—N4B—C6B	103.7 (12)
N6—C4—N9	120.58 (11)	C4B—N5B—N4B	96.8 (12)
N6—C5—N7	138.53 (12)	C4B—N6B—C5B	101.5 (14)
N6—C5—N4	110.46 (11)	C5B—N7B—N8B	108.3 (13)
N7—C5—N4	111.01 (12)	C6B—N8B—N7B	106.1 (14)
N8—C6—N4	110.44 (12)	O2B—N9B—O3B	120.3 (19)
N8—C6—N10	124.41 (12)	O2B—N9B—C4B	120.9 (16)
N4—C6—N10	125.13 (12)	O3B—N9B—C4B	118.7 (16)
C6—N4—C5	104.46 (11)	O4B—N10B—O5B	121 (2)
C6—N4—N5	144.23 (12)	O4B—N10B—C6B	120.0 (17)
C5—N4—N5	111.32 (11)	O5B—N10B—C6B	119.2 (19)
N1—C1—C2—N3	−179.67 (14)	N8—C6—N10—O4	179.98 (12)
O1—C1—C2—N3	−0.31 (13)	N4—C6—N10—O4	−1.42 (19)
O1—N2—N3—C2	−0.24 (13)	N8—C6—N10—O5	0.32 (19)
O1—N2—N3—C3	179.57 (10)	N4—C6—N10—O5	178.92 (13)

C1—C2—N3—N2	0.36 (14)	N7B—C5B—N4B—N5B	180 (2)
C1—C2—N3—C3	−179.44 (12)	N6B—C5B—N4B—N5B	2 (3)
N1—C1—O1—N2	179.66 (11)	N7B—C5B—N4B—C6B	−1 (3)
C2—C1—O1—N2	0.19 (13)	N6B—C5B—N4B—C6B	−179 (2)
N3—N2—O1—C1	0.02 (12)	N8B—C6B—N4B—N5B	178 (3)
N8—C6—N4—C5	0.43 (14)	N10B—C6B—N4B—N5B	−2 (5)
N10—C6—N4—C5	−178.33 (12)	N8B—C6B—N4B—C5B	0 (3)
N8—C6—N4—N5	−179.40 (17)	N10B—C6B—N4B—C5B	180 (2)
N10—C6—N4—N5	1.8 (3)	N6B—C4B—N5B—N4B	−1 (3)
N6—C5—N4—C6	179.40 (11)	N9B—C4B—N5B—N4B	−177 (2)
N7—C5—N4—C6	−0.43 (14)	C5B—N4B—N5B—C4B	−1 (3)
N6—C5—N4—N5	−0.71 (15)	C6B—N4B—N5B—C4B	−179 (4)
N7—C5—N4—N5	179.46 (10)	N5B—C4B—N6B—C5B	2 (3)
N6—C4—N5—N4	−0.29 (15)	N9B—C4B—N6B—C5B	178 (2)
N9—C4—N5—N4	−179.99 (10)	N7B—C5B—N6B—C4B	−179 (3)
C6—N4—N5—C4	−179.61 (18)	N4B—C5B—N6B—C4B	−3 (3)
C5—N4—N5—C4	0.56 (13)	N6B—C5B—N7B—N8B	179 (3)
N5—C4—N6—C5	−0.10 (15)	N4B—C5B—N7B—N8B	3 (3)
N9—C4—N6—C5	179.59 (11)	N4B—C6B—N8B—N7B	2 (3)
N7—C5—N6—C4	−179.77 (15)	N10B—C6B—N8B—N7B	−178 (2)
N4—C5—N6—C4	0.46 (13)	C5B—N7B—N8B—C6B	−2 (3)
N6—C5—N7—N8	−179.49 (15)	N6B—C4B—N9B—O2B	−179 (2)
N4—C5—N7—N8	0.28 (14)	N5B—C4B—N9B—O2B	−3 (3)
N4—C6—N8—N7	−0.28 (14)	N6B—C4B—N9B—O3B	4 (4)
N10—C6—N8—N7	178.50 (11)	N5B—C4B—N9B—O3B	−180 (2)
C5—N7—N8—C6	0.00 (14)	N8B—C6B—N10B—O4B	−178 (2)
N5—C4—N9—O2	1.68 (17)	N4B—C6B—N10B—O4B	3 (4)
N6—C4—N9—O2	−178.02 (12)	N8B—C6B—N10B—O5B	−3 (4)
N5—C4—N9—O3	−178.61 (14)	N4B—C6B—N10B—O5B	177 (3)
N6—C4—N9—O3	1.69 (19)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···N6^i	0.95	2.42	3.2951 (17)	154
C2—H2···N7B^i	0.95	2.58	3.111 (15)	116
C2—H2···N8B^i	0.95	1.95	2.789 (18)	147
C3—H3A···O4^{ii}	0.98	2.60	3.4557 (18)	146
C3—H3C···O2B^{iii}	0.98	2.05	2.88 (2)	140
C3—H3C···O3B^{iii}	0.98	2.45	3.38 (2)	159
C3—H3C···N9B^{iii}	0.98	2.59	3.544 (16)	165
N1—H1A···O5^{iv}	0.854 (19)	2.342 (19)	3.1010 (17)	148.3 (15)
N1—H1A···N8^{iv}	0.854 (19)	2.330 (18)	3.0269 (17)	139.1 (15)
N1—H1A···O3B^{iv}	0.854 (19)	2.58 (3)	3.29 (2)	141.3 (16)
N1—H1A···N6B^{iv}	0.854 (19)	2.56 (3)	3.342 (17)	152.5 (16)
N1—H1B···N7^i	0.898 (19)	2.02 (2)	2.9131 (16)	173.9 (17)
N1—H1B···N7B^i	0.898 (19)	1.97 (2)	2.748 (15)	144.0 (17)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1, *y*, *z*; (iv) −*x*, −*y*+1, −*z*+2.

**Compound 6**
CCDC-2035560
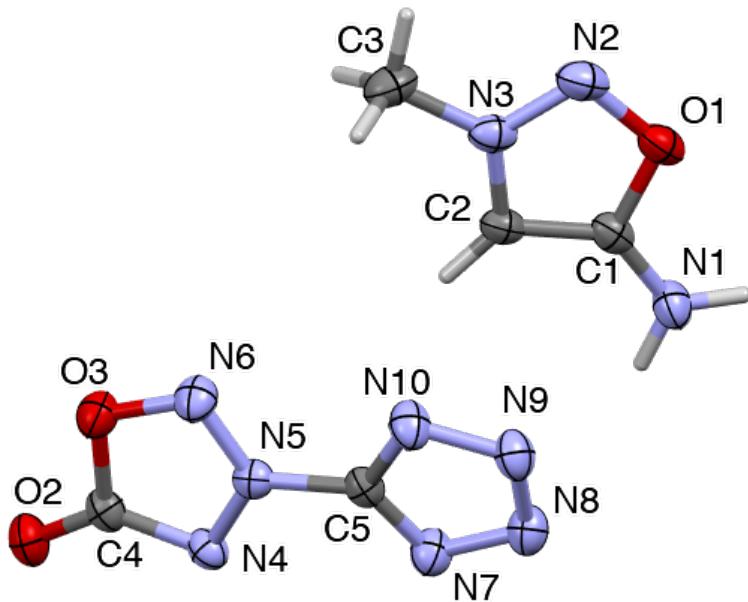
Fig. 5 Molecular unit of 5-amino-3-methyl-1,2,3-oxadiazolium TAZ (**6**). Ellipsoids are drawn at the 50% probability level.

Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$C_2N_7O_2 \cdot C_3H_6N_3O$
M_r	254.20
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, b, c (Å)	5.2488 (8), 13.9673 (14), 14.1051 (18)
V (Å³)	1034.1 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	0.14
Crystal size (mm)	$0.21 \times 0.11 \times 0.05$
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.607, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19772, 3434, 2584
R_{int}	0.073
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.736
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.097, 1.01
No. of reflections	3434
No. of parameters	164
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å⁻³)	0.27, −0.21
Absolute structure	Flack x determined using 889 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	0.3 (8)

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1146 (Hübschle *et al.*, 2011).

Table 2

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1A⋯N8^i	0.88	2.09	2.942 (3)	164
N1—H1B⋯N9	0.88	2.08	2.903 (3)	156
C2—H2⋯O2^{ii}	0.95	2.54	3.254 (3)	132
C2—H2⋯N10	0.95	2.54	3.332 (3)	140
C3—H3A⋯N7^{iii}	0.98	2.53	3.493 (3)	169
C3—H3B⋯N7^{iv}	0.98	2.50	3.250 (3)	133
C3—H3C⋯O2^v	0.98	2.59	3.110 (3)	113

Symmetry codes: (i) x−1/2, −y+3/2, −z+2; (ii) x−1/2, −y+3/2, −z+1; (iii) −x, y−1/2, −z+3/2; (iv) −x+1, y−1/2, −z+3/2; (v) x−3/2, −y+3/2, −z+1.

References

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Figure 1

supporting information

Title

Computing details

Data collection: Apex3 v2019.1-0 (Bruker, 2019); cell refinement: *SAINT* V8.40A (Bruker, 2019); data reduction: *SAINT* V8.40A (Bruker, 2019); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1146 (Hübschle *et al.*, 2011).

(G117d_MSI_TAZ_EtOH_0m)

Crystal data

$C_2N_7O_2 \cdot C_3H_6N_3O$
$M_r = 254.20$
Orthorhombic, $P2_12_12_1$
$a = 5.2488\,(8)$ Å
$b = 13.9673\,(14)$ Å
$c = 14.1051\,(18)$ Å
$V = 1034.1\,(2)$ Å^3
$Z = 4$
$F(000) = 520$

$D_x = 1.633$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5415 reflections
$\theta = 2.9–30.6°$
$\mu = 0.14$ mm^{-1}
$T = 150$ K
Fragment, colourless
$0.21 \times 0.11 \times 0.05$ mm

Data collection

Bruker AXS D8 Quest
diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Radiation source: fine focus sealed tube X-ray source
Triumph curved graphite crystal monochromator
Detector resolution: 7.4074 pixels mm^{-1}
ω and phi scans

Absorption correction: multi-scan
SADABS 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
$T_{min} = 0.607$, $T_{max} = 0.746$
19772 measured reflections
3434 independent reflections
2584 reflections with $I > 2\sigma(I)$
$R_{int} = 0.073$
$\theta_{max} = 31.5°$, $\theta_{min} = 2.9°$
$h = -7 \rightarrow 7$
$k = -18 \rightarrow 20$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.097$
$S = 1.01$
3434 reflections
164 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0344P)^2 + 0.2762P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: Flack x determined using 889 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter: 0.3 (8)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\mathring{A}^2$)

	x	y	z	U_{iso}*/U_{eq}
O1	−0.1296 (3)	0.56228 (12)	0.94960 (12)	0.0332 (4)
O2	0.7501 (4)	0.95350 (12)	0.40370 (12)	0.0373 (4)
O3	0.4686 (3)	0.84396 (12)	0.46206 (12)	0.0330 (4)
N1	0.2371 (4)	0.65170 (13)	0.95988 (14)	0.0331 (4)
H1A	0.214738	0.655591	1.021592	0.040*
H1B	0.369504	0.679452	0.933264	0.040*
N2	−0.2753 (4)	0.51637 (15)	0.88088 (16)	0.0360 (5)
N3	−0.1549 (4)	0.53455 (13)	0.80265 (15)	0.0290 (4)
N4	0.7796 (4)	0.89339 (12)	0.55828 (13)	0.0260 (4)
N5	0.6223 (3)	0.83078 (12)	0.59714 (13)	0.0236 (4)
N6	0.4369 (4)	0.79859 (14)	0.54701 (14)	0.0319 (4)
N7	0.7944 (4)	0.85058 (13)	0.75210 (14)	0.0310 (4)
N8	0.7479 (4)	0.80798 (13)	0.83542 (13)	0.0318 (4)
N9	0.5785 (4)	0.73962 (14)	0.82339 (14)	0.0322 (4)
N10	0.5076 (4)	0.73465 (14)	0.73228 (14)	0.0323 (5)
C1	0.0730 (4)	0.60454 (15)	0.90759 (16)	0.0268 (4)
C2	0.0565 (4)	0.58722 (15)	0.81171 (17)	0.0265 (4)
H2	0.169215	0.607911	0.763168	0.032*
C3	−0.2648 (5)	0.49785 (19)	0.7134 (2)	0.0386 (6)
H3A	−0.425035	0.464566	0.726935	0.058*
H3B	−0.144703	0.453213	0.683759	0.058*
H3C	−0.297435	0.551426	0.670190	0.058*
C4	0.6861 (4)	0.90443 (15)	0.46992 (16)	0.0261 (4)
C5	0.6452 (4)	0.80346 (15)	0.69362 (15)	0.0238 (4)

Atomic displacement parameters ($\mathring{A}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0278 (8)	0.0351 (8)	0.0366 (9)	0.0031 (7)	0.0090 (7)	0.0086 (7)
O2	0.0448 (10)	0.0399 (9)	0.0272 (8)	−0.0006 (9)	0.0041 (8)	0.0059 (7)
O3	0.0377 (9)	0.0329 (8)	0.0284 (9)	−0.0046 (7)	−0.0053 (7)	0.0020 (7)
N1	0.0393 (11)	0.0350 (10)	0.0250 (9)	−0.0044 (9)	0.0053 (9)	0.0012 (8)
N2	0.0252 (9)	0.0365 (10)	0.0463 (12)	0.0003 (8)	0.0048 (9)	0.0093 (9)
N3	0.0228 (9)	0.0259 (9)	0.0383 (11)	0.0009 (7)	0.0004 (8)	0.0067 (8)
N4	0.0274 (9)	0.0236 (8)	0.0270 (9)	−0.0032 (8)	0.0043 (8)	0.0001 (7)
N5	0.0244 (9)	0.0197 (8)	0.0267 (9)	0.0001 (7)	0.0003 (7)	−0.0018 (7)
N6	0.0359 (10)	0.0298 (9)	0.0300 (10)	−0.0082 (9)	−0.0034 (9)	0.0008 (8)
N7	0.0366 (11)	0.0279 (9)	0.0284 (10)	−0.0045 (8)	−0.0018 (8)	0.0019 (7)
N8	0.0398 (11)	0.0286 (9)	0.0270 (10)	−0.0002 (9)	−0.0015 (9)	0.0006 (7)
N9	0.0417 (11)	0.0288 (9)	0.0262 (10)	−0.0023 (9)	0.0033 (8)	0.0047 (8)
N10	0.0405 (12)	0.0283 (9)	0.0279 (10)	−0.0087 (9)	0.0019 (8)	0.0023 (8)
C1	0.0263 (10)	0.0230 (9)	0.0310 (11)	0.0036 (8)	0.0061 (9)	0.0057 (9)
C2	0.0211 (10)	0.0252 (10)	0.0334 (12)	0.0003 (8)	0.0030 (9)	0.0043 (9)

C3	0.0289 (12)	0.0392 (12)	0.0477 (15)	−0.0040 (11)	−0.0087 (11)	0.0020 (11)
C4	0.0302 (11)	0.0215 (9)	0.0264 (11)	0.0014 (8)	0.0044 (8)	−0.0016 (8)
C5	0.0267 (10)	0.0202 (9)	0.0245 (10)	0.0025 (8)	0.0033 (9)	0.0009 (8)

Geometric parameters (Å, º)

O1—C1	1.353 (3)	N5—N6	1.284 (3)
O1—N2	1.391 (3)	N5—C5	1.418 (3)
O2—C4	1.206 (3)	N7—C5	1.314 (3)
O3—N6	1.366 (3)	N7—N8	1.340 (3)
O3—C4	1.425 (3)	N8—N9	1.315 (3)
N1—C1	1.311 (3)	N9—N10	1.340 (3)
N1—H1A	0.8800	N10—C5	1.320 (3)
N1—H1B	0.8800	C1—C2	1.377 (3)
N2—N3	1.297 (3)	C2—H2	0.9500
N3—C2	1.338 (3)	C3—H3A	0.9800
N3—C3	1.477 (3)	C3—H3B	0.9800
N4—N5	1.322 (2)	C3—H3C	0.9800
N4—C4	1.348 (3)		

C1—O1—N2	109.16 (18)	N1—C1—O1	119.3 (2)
N6—O3—C4	107.73 (17)	N1—C1—C2	133.0 (2)
C1—N1—H1A	120.0	O1—C1—C2	107.7 (2)
C1—N1—H1B	120.0	N3—C2—C1	104.1 (2)
H1A—N1—H1B	120.0	N3—C2—H2	128.0
N3—N2—O1	103.57 (18)	C1—C2—H2	128.0
N2—N3—C2	115.5 (2)	N3—C3—H3A	109.5
N2—N3—C3	117.9 (2)	N3—C3—H3B	109.5
C2—N3—C3	126.6 (2)	H3A—C3—H3B	109.5
N5—N4—C4	103.40 (18)	N3—C3—H3C	109.5
N6—N5—N4	118.47 (19)	H3A—C3—H3C	109.5
N6—N5—C5	119.87 (18)	H3B—C3—H3C	109.5
N4—N5—C5	121.54 (18)	O2—C4—N4	132.8 (2)
N5—N6—O3	103.19 (18)	O2—C4—O3	120.0 (2)
C5—N7—N8	102.67 (19)	N4—C4—O3	107.20 (18)
N9—N8—N7	109.43 (19)	N7—C5—N10	115.6 (2)
N8—N9—N10	110.44 (18)	N7—C5—N5	121.18 (19)
C5—N10—N9	101.90 (19)	N10—C5—N5	123.1 (2)

C1—O1—N2—N3	−0.7 (2)	N1—C1—C2—N3	180.0 (2)
O1—N2—N3—C2	0.4 (2)	O1—C1—C2—N3	−0.6 (2)
O1—N2—N3—C3	−178.28 (18)	N5—N4—C4—O2	178.8 (2)
C4—N4—N5—N6	0.0 (2)	N5—N4—C4—O3	−0.2 (2)
C4—N4—N5—C5	−176.13 (18)	N6—O3—C4—O2	−178.74 (19)
N4—N5—N6—O3	0.3 (2)	N6—O3—C4—N4	0.4 (2)
C5—N5—N6—O3	176.48 (17)	N8—N7—C5—N10	0.0 (3)
C4—O3—N6—N5	−0.4 (2)	N8—N7—C5—N5	175.47 (19)
C5—N7—N8—N9	0.0 (3)	N9—N10—C5—N7	0.0 (3)
N7—N8—N9—N10	0.0 (3)	N9—N10—C5—N5	−175.4 (2)
N8—N9—N10—C5	0.0 (3)	N6—N5—C5—N7	−164.5 (2)
N2—O1—C1—N1	−179.66 (19)	N4—N5—C5—N7	11.6 (3)
N2—O1—C1—C2	0.9 (2)	N6—N5—C5—N10	10.6 (3)

N2—N3—C2—C1	0.1 (2)	N4—N5—C5—N10	−173.3 (2)
C3—N3—C2—C1	178.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$A\cdots$N8[i]	0.88	2.09	2.942 (3)	164
N1—H1$B\cdots$N9	0.88	2.08	2.903 (3)	156
C2—H2$\cdots$O2[ii]	0.95	2.54	3.254 (3)	132
C2—H2$\cdots$N10	0.95	2.54	3.332 (3)	140
C3—H3$A\cdots$N7[iii]	0.98	2.53	3.493 (3)	169
C3—H3$B\cdots$N7[iv]	0.98	2.50	3.250 (3)	133
C3—H3$C\cdots$O2[v]	0.98	2.59	3.110 (3)	113

Symmetry codes: (i) $x-1/2$, $-y+3/2$, $-z+2$; (ii) $x-1/2$, $-y+3/2$, $-z+1$; (iii) $-x$, $y-1/2$, $-z+3/2$; (iv) $-x+1$, $y-1/2$, $-z+3/2$; (v) $x-3/2$, $-y+3/2$, $-z+1$.

Compound 7
CCDC-2025853
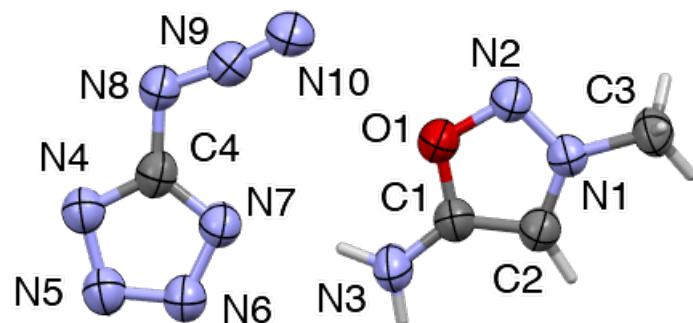
**Fig. 6** Molecular unit of 5-amino-3-methyl-1,2,3-oxadiazolium azidotetrazolate (**7**). Ellipsoids are drawn at the 50% probability level.

Title

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Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$CN_7 \cdot C_3H_6N_3O$
M_r	210.19
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	8.4296 (13), 5.5977 (9), 19.058 (3)
β (°)	96.392 (10)
V (Å^3)	893.7 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.07
Crystal size (mm)	$0.15 \times 0.02 \times 0.01$
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonIII_C14 charge-integrating and photon counting pixel array detector
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.502, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7434, 1744, 735
R_{int}	0.182
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.092, 0.301, 0.97
No. of reflections	1744
No. of parameters	137
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.28, −0.45

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

Table 2

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N3—H3$A$$\cdots$N6	0.88	2.69	3.417 (7)	141
N3—H3$A$$\cdots$N7	0.88	2.03	2.898 (7)	169
N3—H3$B$$\cdots$N6[i]	0.88	2.03	2.883 (8)	164
C3—H3$C$$\cdots$N10[ii]	0.98	2.63	3.365 (9)	132
C3—H3$D$$\cdots$N4[iii]	0.98	2.47	3.419 (9)	163
C3—H3$D$$\cdots$N5[iii]	0.98	2.53	3.429 (9)	153
C3—H3$E$$\cdots$N5[iv]	0.98	2.67	3.313 (8)	123

Symmetry codes: (i) $-x+2$, $-y+2$, $-z+1$; (ii) $-x+1$, $-y$, $-z+1$; (iii) $x-1/2$, $-y+3/2$, $z+1/2$; (iv) $-x+2$, $-y+1$, $-z+1$.

References

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). J. Appl. Cryst., 37, 335–338.

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CSD: Groom, C. R. & Allen, F. H. (2014). Angew. Chem. Int. Ed., 53, 662–671.

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Spek, A. L. (2003). J. Appl. Cryst., 36, 7–13.

Figure 1

supporting information

Title

Computing details

Data collection: Apex3 v2019.1-0 (Bruker, 2019); cell refinement: *SAINT* V8.40A (Bruker, 2019); data reduction: *SAINT* V8.40A (Bruker, 2019); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

(G117d_MSI_TAZ_0m)

Crystal data

$CN_7 \cdot C_3H_6N_3O$
$M_r = 210.19$
Monoclinic, $P2_1/n$
$a = 8.4296 (13)$ Å
$b = 5.5977 (9)$ Å
$c = 19.058 (3)$ Å
$\beta = 96.392 (10)°$
$V = 893.7 (2)$ Å^3
$Z = 4$

$F(000) = 432$
$D_x = 1.562$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 719 reflections
$\theta = 5.5–58.2°$
$\mu = 1.07$ mm^{-1}
$T = 150$ K
Needle, colourless
$0.15 \times 0.02 \times 0.01$ mm

Data collection

Bruker AXS D8 Quest
    diffractometer with PhotonIII_C14 charge-integrating
    and photon counting pixel array detector
Radiation source: I-mu-S microsource X-ray tube
Laterally graded multilayer (Goebel) mirror
    monochromator
Detector resolution: 7.4074 pixels mm^{-1}
ω and phi scans

Absorption correction: multi-scan
    SADABS 2016/2: Krause, L., Herbst-Irmer, R.,
    Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015)
    3-10
$T_{min} = 0.502$, $T_{max} = 0.754$
7434 measured reflections
1744 independent reflections
735 reflections with $I > 2\sigma(I)$
$R_{int} = 0.182$
$\theta_{max} = 72.2°$, $\theta_{min} = 5.5°$
$h = -10 \rightarrow 10$
$k = -6 \rightarrow 6$
$l = -23 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.092$
$wR(F^2) = 0.301$
$S = 0.97$
1744 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct
    methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring
    sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1226P)^2]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.6899 (5)	0.4107 (9)	0.5096 (2)	0.0622 (12)
N1	0.6027 (5)	0.3866 (10)	0.6086 (2)	0.0520 (12)
N2	0.5985 (6)	0.2701 (10)	0.5492 (3)	0.0587 (14)
N3	0.8367 (6)	0.7528 (10)	0.5179 (3)	0.0641 (15)
H3A	0.857767	0.730234	0.474175	0.077*
H3B	0.875772	0.878161	0.541741	0.077*
N4	1.0387 (6)	0.7372 (10)	0.2748 (3)	0.0584 (14)
N5	1.1048 (6)	0.9085 (11)	0.3191 (3)	0.0623 (15)
N6	1.0510 (6)	0.8853 (11)	0.3809 (3)	0.0606 (14)
N7	0.9482 (6)	0.7013 (10)	0.3802 (3)	0.0570 (14)
N8	0.8535 (6)	0.4220 (10)	0.2865 (3)	0.0602 (14)
N9	0.7881 (6)	0.3111 (11)	0.3319 (3)	0.0589 (14)
N10	0.7189 (7)	0.1998 (11)	0.3671 (3)	0.0691 (16)
C1	0.7477 (7)	0.6003 (13)	0.5473 (3)	0.0553 (15)
C2	0.6886 (7)	0.5854 (12)	0.6126 (3)	0.0548 (15)
H2	0.705933	0.693206	0.651149	0.066*
C3	0.5200 (7)	0.2786 (12)	0.6649 (3)	0.0612 (17)
H3C	0.413256	0.226386	0.645225	0.092*
H3D	0.510613	0.396753	0.702134	0.092*
H3E	0.581078	0.140699	0.684732	0.092*
C4	0.9454 (7)	0.6177 (13)	0.3152 (3)	0.0554 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.074 (3)	0.065 (3)	0.050 (2)	−0.012 (2)	0.0158 (19)	−0.007 (2)
N1	0.054 (3)	0.053 (3)	0.050 (3)	−0.005 (2)	0.012 (2)	−0.001 (2)
N2	0.069 (3)	0.056 (4)	0.054 (3)	−0.006 (2)	0.018 (2)	−0.005 (2)
N3	0.079 (3)	0.064 (4)	0.052 (3)	−0.012 (3)	0.022 (2)	0.002 (3)
N4	0.059 (3)	0.063 (4)	0.054 (3)	−0.003 (2)	0.010 (2)	0.002 (3)
N5	0.064 (3)	0.067 (4)	0.057 (3)	−0.004 (3)	0.012 (2)	0.004 (3)
N6	0.066 (3)	0.064 (4)	0.053 (3)	−0.005 (3)	0.013 (2)	0.000 (3)
N7	0.063 (3)	0.056 (3)	0.054 (3)	−0.003 (2)	0.015 (2)	−0.003 (2)
N8	0.070 (3)	0.062 (4)	0.051 (3)	−0.008 (3)	0.017 (2)	−0.005 (3)
N9	0.063 (3)	0.061 (4)	0.053 (3)	−0.005 (3)	0.009 (2)	−0.005 (3)
N10	0.078 (4)	0.061 (4)	0.069 (3)	−0.014 (3)	0.014 (3)	−0.005 (3)
C1	0.056 (3)	0.061 (4)	0.049 (3)	−0.008 (3)	0.010 (2)	0.000 (3)
C2	0.061 (3)	0.055 (4)	0.050 (3)	−0.002 (3)	0.011 (3)	−0.002 (3)
C3	0.072 (4)	0.055 (4)	0.060 (4)	−0.005 (3)	0.024 (3)	0.005 (3)
C4	0.056 (3)	0.062 (4)	0.049 (3)	0.006 (3)	0.010 (2)	0.000 (3)

Geometric parameters (Å, º)

O1—C1	1.343 (8)	N6—N7	1.345 (7)
O1—N2	1.382 (7)	N7—C4	1.322 (8)
N1—N2	1.304 (7)	N8—N9	1.241 (7)
N1—C2	1.325 (8)	N8—C4	1.416 (8)
N1—C3	1.472 (7)	N9—N10	1.125 (8)
N3—C1	1.304 (8)	C1—C2	1.392 (8)
N3—H3A	0.8800	C2—H2	0.9500
N3—H3B	0.8800	C3—H3C	0.9800
N4—C4	1.338 (8)	C3—H3D	0.9800
N4—N5	1.356 (7)	C3—H3E	0.9800
N5—N6	1.314 (7)		
C1—O1—N2	110.4 (4)	N3—C1—C2	134.7 (6)
N2—N1—C2	115.5 (5)	O1—C1—C2	106.6 (5)
N2—N1—C3	117.3 (5)	N1—C2—C1	104.3 (5)
C2—N1—C3	127.1 (5)	N1—C2—H2	127.8
N1—N2—O1	103.1 (4)	C1—C2—H2	127.8
C1—N3—H3A	120.0	N1—C3—H3C	109.5
C1—N3—H3B	120.0	N1—C3—H3D	109.5
H3A—N3—H3B	120.0	H3C—C3—H3D	109.5
C4—N4—N5	102.9 (5)	N1—C3—H3E	109.5
N6—N5—N4	109.2 (5)	H3C—C3—H3E	109.5
N5—N6—N7	110.7 (5)	H3D—C3—H3E	109.5
C4—N7—N6	103.0 (5)	N7—C4—N4	114.3 (6)
N9—N8—C4	112.6 (5)	N7—C4—N8	126.0 (5)
N10—N9—N8	172.6 (6)	N4—C4—N8	119.8 (5)
N3—C1—O1	118.6 (5)		
C2—N1—N2—O1	−1.0 (7)	C3—N1—C2—C1	176.6 (6)
C3—N1—N2—O1	−177.8 (5)	N3—C1—C2—N1	178.8 (7)
C1—O1—N2—N1	1.5 (6)	O1—C1—C2—N1	0.9 (6)
C4—N4—N5—N6	0.0 (6)	N6—N7—C4—N4	−0.3 (7)
N4—N5—N6—N7	−0.2 (7)	N6—N7—C4—N8	−179.6 (6)
N5—N6—N7—C4	0.3 (7)	N5—N4—C4—N7	0.2 (7)
N2—O1—C1—N3	−179.9 (5)	N5—N4—C4—N8	179.5 (5)
N2—O1—C1—C2	−1.6 (6)	N9—N8—C4—N7	−8.9 (9)
N2—N1—C2—C1	0.0 (7)	N9—N8—C4—N4	171.9 (6)

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3—H3A⋯N6	0.88	2.69	3.417 (7)	141
N3—H3A⋯N7	0.88	2.03	2.898 (7)	169
N3—H3B⋯N6[i]	0.88	2.03	2.883 (8)	164
C3—H3C⋯N10[ii]	0.98	2.63	3.365 (9)	132
C3—H3D⋯N4[iii]	0.98	2.47	3.419 (9)	163
C3—H3D⋯N5[iii]	0.98	2.53	3.429 (9)	153
C3—H3E⋯N5[iv]	0.98	2.67	3.313 (8)	123

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*+1; (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*−1/2, −*y*+3/2, *z*+1/2; (iv) −*x*+2, −*y*+1, −*z*+1.

Compound 8: 3-methyl-1,2,3-oxadiazolium nitrosoamide

Compound 8
CCDC-2025852
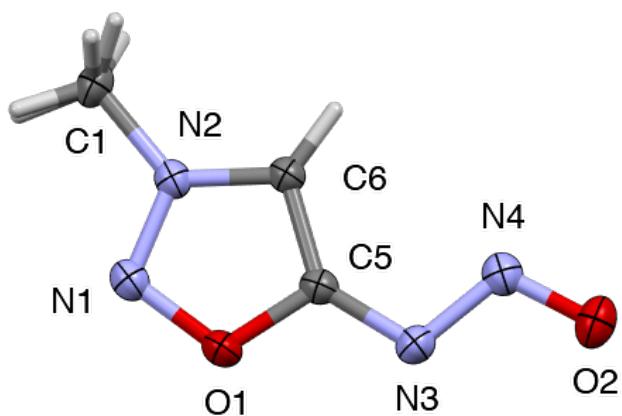
Fig. 7 Molecular unit of 3-methyl-1,2,3-oxadiazolium nitrosoamide (**8**). Ellipsoids are drawn at the 50% probability level. Disorder of methyl H atoms is symmetry imposed by a mirror plane bisecting the molecule.

Title

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Department of Chemistry, Purdue University, 560 Oval Dr., W. Lafayette, IN 47907-2084, USA

Correspondence email: zeller4@purdue.edu

Abstract

Table 1

Experimental details

Crystal data	
Chemical formula	$C_3H_4N_4O_2$
M_r	128.10
Crystal system, space group	Orthorhombic, $Cmc2_1$
Temperature (K)	150
a, b, c (Å)	6.1158 (7), 9.1928 (9), 9.3984 (10)
V (Å^3)	528.39 (10)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.14
Crystal size (mm)	$0.31 \times 0.22 \times 0.20$
Data collection	
Diffractometer	Bruker AXS D8 Quest diffractometer with PhotonII charge-integrating pixel array detector (CPAD)
Absorption correction	Multi-scan *SADABS* 2016/2: Krause, L., Herbst-Irmer, R., Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015) 3-10
T_{min}, T_{max}	0.630, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4289, 1077, 989
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.770
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.091, 1.07
No. of reflections	1077
No. of parameters	56
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.27, −0.22
Absolute structure	Flack x determined using 434 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	−0.1 (7)

Computer programs: Apex3 v2019.1-0 (Bruker, 2019), *SAINT* V8.40A (Bruker, 2019), *SHELXS97* (Sheldrick, 2008), *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

Table 2

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C1—H1$B\cdots$O2^{i}	0.98	2.51	3.458 (3)	162
C6—H6$\cdots$N3^{ii}	0.95	2.32	3.269 (2)	179

Symmetry codes: (i) x, y+1, z; (ii) $-x$, $-y$+1, z+1/2.

Acknowledgements

Funding information

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Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). J. Appl. Cryst., 37, 335–338.

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publCIF: Westrip, S. P. (2010). J. Appl. Cryst., 43, 920–925.

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Spek, A. L. (2003). J. Appl. Cryst., 36, 7–13.

Figure 1

supporting information

Title

Computing details

Data collection: Apex3 v2019.1-0 (Bruker, 2019); cell refinement: *SAINT* V8.40A (Bruker, 2019); data reduction: *SAINT* V8.40A (Bruker, 2019); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018*/3 (Sheldrick, 2015, 2018), SHELXLE Rev1117 (Hübschle *et al.*, 2011).

(G117c3_MSI_NO2BF4_0m)

Crystal data

$C_3H_4N_4O_2$
$M_r = 128.10$
Orthorhombic, $Cmc2_1$
$a = 6.1158 (7)$ Å
$b = 9.1928 (9)$ Å
$c = 9.3984 (10)$ Å
$V = 528.39 (10)$ Å^3
$Z = 4$
$F(000) = 264$

$D_x = 1.610$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3960 reflections
$\theta = 4.0–33.1°$
$\mu = 0.14$ mm^{-1}
$T = 150$ K
Block, yellow
$0.31 \times 0.22 \times 0.20$ mm

Data collection

Bruker AXS D8 Quest
    diffractometer with PhotonII charge-integrating pixel
    array detector (CPAD)
Radiation source: fine focus sealed tube X-ray source
Triumph curved graphite crystal monochromator
Detector resolution: 7.4074 pixels mm^{-1}
ω and phi scans

Absorption correction: multi-scan
    SADABS 2016/2: Krause, L., Herbst-Irmer, R.,
    Sheldrick G.M. & Stalke D., J. Appl. Cryst. 48 (2015)
    3-10
$T_{min} = 0.630$, $T_{max} = 0.747$
4289 measured reflections
1077 independent reflections
989 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 33.2°$, $\theta_{min} = 4.0°$
$h = -8\rightarrow9$
$k = -14\rightarrow14$
$l = -13\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.091$
$S = 1.07$
1077 reflections
56 parameters
1 restraint
Primary atom site location: structure-invariant direct
    methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring
    sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2]$
    where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
Absolute structure: Flack x determined using 434
    quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons, Flack and
    Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter: −0.1 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
O1	0.000000	0.72558 (15)	−0.12018 (15)	0.0265 (3)	
O2	0.000000	0.25532 (16)	−0.0167 (2)	0.0333 (4)	
N1	0.000000	0.85694 (18)	−0.05157 (17)	0.0263 (4)	
N2	0.000000	0.82298 (15)	0.08329 (16)	0.0217 (3)	
N3	0.000000	0.48009 (19)	−0.07896 (16)	0.0259 (4)	
N4	0.000000	0.38404 (18)	0.0260 (2)	0.0267 (3)	
C1	0.000000	0.9418 (2)	0.1867 (2)	0.0292 (4)	
H1A	−0.144379	0.948728	0.231439	0.044*	0.5
H1B	0.033664	1.033517	0.138201	0.044*	0.5
H1C	0.110714	0.922947	0.259789	0.044*	0.5
C5	0.000000	0.6148 (2)	−0.02386 (17)	0.0212 (3)	
C6	0.000000	0.67869 (18)	0.10978 (19)	0.0216 (4)	
H6	0.000000	0.631530	0.199718	0.026*	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0372 (8)	0.0241 (6)	0.0182 (6)	0.000	0.000	0.0030 (6)
O2	0.0360 (8)	0.0224 (7)	0.0415 (9)	0.000	0.000	−0.0040 (5)
N1	0.0326 (8)	0.0231 (7)	0.0231 (8)	0.000	0.000	0.0038 (6)
N2	0.0241 (7)	0.0197 (7)	0.0212 (8)	0.000	0.000	0.0023 (6)
N3	0.0350 (8)	0.0211 (7)	0.0217 (7)	0.000	0.000	−0.0026 (6)
N4	0.0298 (7)	0.0241 (7)	0.0261 (7)	0.000	0.000	0.0014 (6)
C1	0.0387 (9)	0.0190 (7)	0.0300 (10)	0.000	0.000	−0.0041 (7)
C5	0.0240 (7)	0.0217 (7)	0.0179 (7)	0.000	0.000	0.0008 (6)
C6	0.0271 (8)	0.0197 (8)	0.0180 (8)	0.000	0.000	0.0008 (6)

Geometric parameters (Å, º)

O1—C5	1.363 (2)	C1—H1A	0.9800
O1—N1	1.369 (2)	C1—H1B	0.9800
O2—N4	1.250 (2)	C1—H1C	0.9800
N1—N2	1.305 (2)	C1—H1A^i	0.980 (13)
N2—C6	1.350 (2)	C1—H1B^i	0.980 (10)
N2—C1	1.462 (2)	C1—H1C^i	0.98 (2)
N3—N4	1.324 (2)	C5—C6	1.386 (3)
N3—C5	1.342 (2)	C6—H6	0.9500
C5—O1—N1	110.26 (14)	N2—C1—H1B^i	109.5 (2)
N2—N1—O1	104.27 (14)	H1A—C1—H1B^i	87.4
N1—N2—C6	114.46 (15)	H1B—C1—H1B^i	24.3
N1—N2—C1	117.82 (15)	H1C—C1—H1B^i	128.6
C6—N2—C1	127.72 (16)	H1A^i—C1—H1B^i	109.5

N4—N3—C5	109.13 (15)	N2—C1—H1C[i]	109.5 (5)
O2—N4—N3	113.08 (19)	H1A—C1—H1C[i]	24.3
N2—C1—H1A	109.5	H1B—C1—H1C[i]	128.6
N2—C1—H1B	109.5	H1C—C1—H1C[i]	87.4
H1A—C1—H1B	109.5	H1A[i]—C1—H1C[i]	109.5
N2—C1—H1C	109.5	H1B[i]—C1—H1C[i]	109.5
H1A—C1—H1C	109.5	N3—C5—O1	115.67 (16)
H1B—C1—H1C	109.5	N3—C5—C6	137.76 (18)
N2—C1—H1A[i]	109.5 (3)	O1—C5—C6	106.58 (15)
H1A—C1—H1A[i]	128.6	N2—C6—C5	104.43 (16)
H1B—C1—H1A[i]	87.4	N2—C6—H6	127.8
H1C—C1—H1A[i]	24.3	C5—C6—H6	127.8
C5—O1—N1—N2	0.000 (1)	N1—O1—C5—N3	180.000 (1)
O1—N1—N2—C6	0.000 (1)	N1—O1—C5—C6	0.000 (1)
O1—N1—N2—C1	180.000 (1)	N1—N2—C6—C5	0.000 (1)
C5—N3—N4—O2	180.000 (1)	C1—N2—C6—C5	180.000 (1)
N4—N3—C5—O1	180.000 (1)	N3—C5—C6—N2	180.000 (1)
N4—N3—C5—C6	0.000 (1)	O1—C5—C6—N2	0.000 (1)

Symmetry code: (i) −x, y, z.

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1B···O2[ii]	0.98	2.51	3.458 (3)	162
C6—H6···N3[iii]	0.95	2.32	3.269 (2)	179

Symmetry codes: (ii) x, y+1, z; (iii) −x, −y+1, z+1/2.