Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Zwitterionic Borane Adducts of N-Heterocyclic Carbenes from Mesomeric Betaines of Uracil.

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Crystallographic data (excluding structure factors) for the structures reported in this work have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 976125 (**25b**), and CCDC 076126 (**25d**). Copies of the data can be obtained free of charge on application to The Director, CCDC, 12 Union Road, Cambridge uB2 1EZ, UK (Fax: int.code+(1223)336-033; e-mail: deposit@ccdc.cam.ac.uk).

10,10-Diethyl-2-(2-hydroxyethyl)-6,8-dioxo-6,7,8,10-tetrahydro-1H-imidazo-[2',1:3,4][1,4,2]diazaborolo[1,5-c]pyrimidinium-10-ide 25b

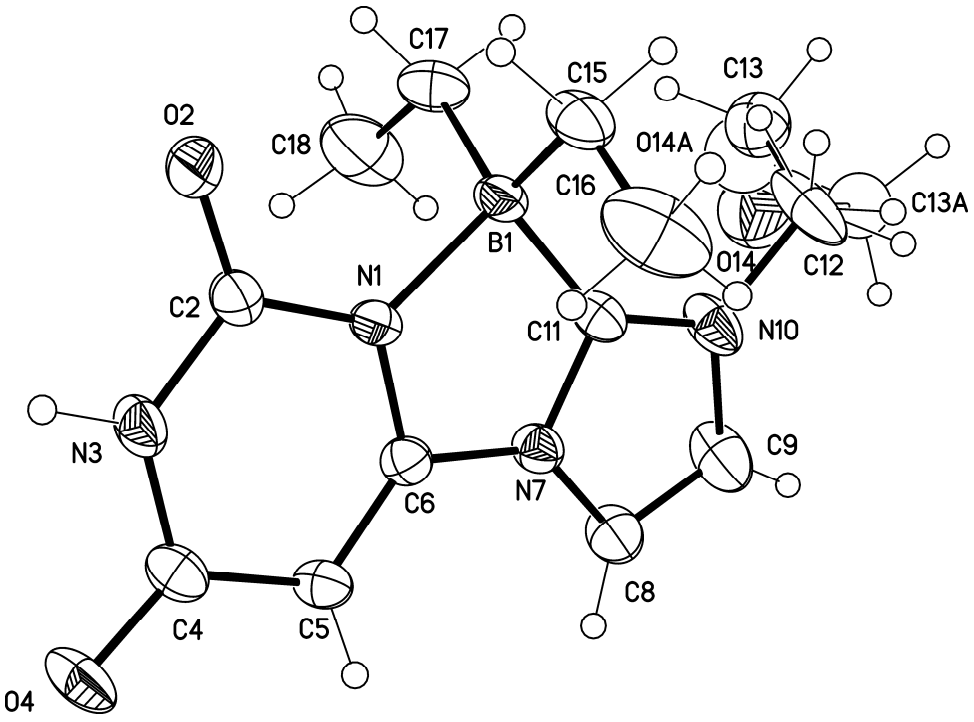


Fig. S1: Molecular structure of **25b** (displacement parameters are drawn at 50% probability level)

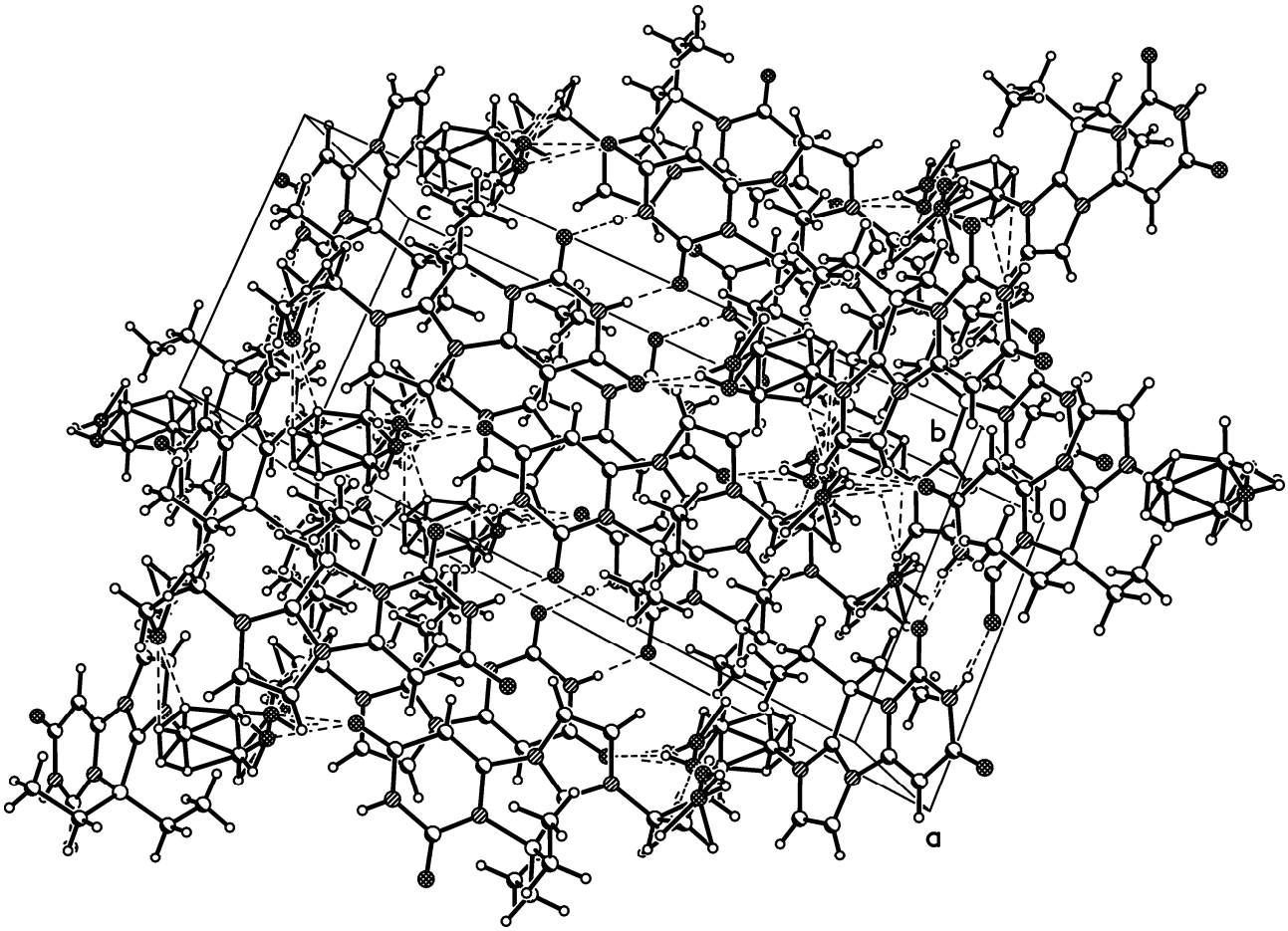


Fig. S2: Packing diagram of **25b**

Crystal data

$C_{13}H_{19}BN_4O_3$	$F(000) = 616$
$M_r = 290.13$	$D_x = 1.339$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.6058$ (4) Å	Cell parameters from 85 reflections
$b = 7.5126$ (3) Å	$\theta = 2.5–25.0°$
$c = 22.4696$ (8) Å	$\mu = 0.10$ mm^{-1}
$\beta = 97.873$ (2)°	$T = 123$ K
$V = 1439.01$ (10) Å^3	Blocks, colourless
$Z = 4$	0.32 × 0.24 × 0.08 mm

Data collection

Bruker-Nonius KappaCCD diffractometer	2748 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.025$
rotation in ϕ and ω, 1° scans	$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
Absorption correction: multi-scan *SADABS* (Shedlrcik, 2008)	$h = -11 \rightarrow 11$
$T_{min} = 0.906$, $T_{max} = 0.993$	$k = -9 \rightarrow 9$
23003 measured reflections	$l = -29 \rightarrow 29$
3291 independent reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.091$	Hydrogen site location: mixed
$wR(F^2) = 0.220$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0745P)^2 + 3.7762P]$ where $P = (F_o^2 + 2F_c^2)/3$
3291 reflections	$(\Delta/\sigma)_{max} < 0.001$
190 parameters	$\Delta\rangle_{max} = 1.40$ e Å^{-3}
9 restraints	$\Delta\rangle_{min} = -1.20$ e Å^{-3}

Computing details

Data collection: Collect; cell refinement: *EVALCCD*; data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXS97*; program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2013); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *publCIF*.

Special details

Experimental. dx = 40 mm, 120 sec./deg., 1 deg., 8 sets, 711 frames, 11965 refl. postref.
Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Refinement. The ethyl-hydroxy group is disordered use of constraints (EADP) and restrains (DFIX, SADI).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
B1	0.7177 (4)	0.6358 (5)	0.36511 (13)	0.0265 (6)	
N1	0.7148 (3)	0.7307 (3)	0.42986 (10)	0.0250 (5)	
C2	0.8345 (3)	0.8262 (4)	0.46082 (13)	0.0289 (6)	
O2	0.9614 (2)	0.8462 (3)	0.44256 (10)	0.0412 (6)	
N3	0.8051 (3)	0.8983 (3)	0.51473 (10)	0.0287 (5)	
H3	0.880 (3)	0.966 (4)	0.5335 (14)	0.034*	
C4	0.6695 (3)	0.8796 (4)	0.54085 (12)	0.0270 (6)	
O4	0.6606 (3)	0.9477 (3)	0.59018 (9)	0.0369 (5)	
C5	0.5458 (3)	0.7830 (4)	0.50549 (11)	0.0251 (6)	
H5	0.4475	0.7641	0.5192	0.030*	
C6	0.5753 (3)	0.7205 (3)	0.45202 (11)	0.0216 (5)	
N7	0.4699 (3)	0.6294 (3)	0.40908 (10)	0.0238 (5)	
C8	0.3117 (3)	0.5859 (4)	0.40233 (14)	0.0337 (7)	
H8	0.2381	0.6134	0.4289	0.040*	
C9	0.2852 (3)	0.4965 (5)	0.35018 (16)	0.0435 (9)	
H9	0.1876	0.4475	0.3329	0.052*	
N10	0.4256 (3)	0.4879 (4)	0.32571 (11)	0.0334 (6)	
C11	0.5374 (3)	0.5710 (4)	0.36176 (11)	0.0243 (6)	
C12	0.4522 (4)	0.4016 (6)	0.26894 (16)	0.0548 (11)	
H12A	0.3806	0.2985	0.2611	0.066*	0.641 (5)
H12B	0.5613	0.3566	0.2729	0.066*	0.641 (5)
H12C	0.4757	0.2741	0.2770	0.066*	0.359 (5)
H12D	0.5456	0.4560	0.2550	0.066*	0.359 (5)
C13	0.4236 (6)	0.5342 (7)	0.2144 (2)	0.0450 (11)*	0.641 (5)
H13A	0.4947	0.6379	0.2216	0.054*	0.641 (5)
H13B	0.4452	0.4741	0.1771	0.054*	0.641 (5)
O14	0.2662 (6)	0.5909 (7)	0.2080 (2)	0.0664 (12)*	0.641 (5)
H14	0.2492	0.6620	0.1790	0.100*	0.641 (5)
C13A	0.3134 (9)	0.4156 (10)	0.2183 (3)	0.0450 (11)*	0.359 (5)
H13C	0.3223	0.3300	0.1854	0.054*	0.359 (5)
H13D	0.2113	0.4000	0.2332	0.054*	0.359 (5)
O14A	0.3379 (12)	0.5955 (10)	0.2006 (4)	0.0664 (12)*	0.359 (5)
H14A	0.2689	0.6235	0.1720	0.100*	0.359 (5)
C15	0.8446 (3)	0.4776 (5)	0.36909 (14)	0.0358 (7)	
H15A	0.8351	0.4183	0.3294	0.043*	
H15B	0.9505	0.5312	0.3766	0.043*	
C16	0.8335 (5)	0.3361 (6)	0.41641 (19)	0.0610 (12)	

H16A	0.9160	0.2471	0.4146	0.092*	
H16B	0.7306	0.2782	0.4090	0.092*	
H16C	0.8468	0.3914	0.4563	0.092*	
C17	0.7351 (5)	0.7837 (5)	0.31457 (15)	0.0471 (9)	
H17A	0.8442	0.8287	0.3211	0.057*	
H17B	0.7194	0.7242	0.2749	0.057*	
C18	0.6268 (7)	0.9403 (5)	0.31178 (19)	0.0686 (14)	
H18A	0.6481	1.0202	0.2794	0.103*	
H18B	0.6435	1.0043	0.3501	0.103*	
H18C	0.5179	0.8990	0.3040	0.103*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0249 (14)	0.0358 (16)	0.0198 (13)	-0.0058 (12)	0.0066 (11)	-0.0091 (12)
N1	0.0233 (11)	0.0316 (12)	0.0212 (10)	-0.0050 (9)	0.0075 (8)	-0.0067 (9)
C2	0.0257 (13)	0.0342 (15)	0.0274 (14)	-0.0052 (11)	0.0057 (10)	-0.0100 (11)
O2	0.0277 (11)	0.0517 (14)	0.0466 (13)	-0.0161 (10)	0.0138 (9)	-0.0245 (11)
N3	0.0230 (11)	0.0364 (13)	0.0259 (12)	-0.0027 (10)	0.0004 (9)	-0.0117 (10)
C4	0.0277 (13)	0.0325 (14)	0.0201 (12)	0.0062 (11)	0.0007 (10)	-0.0011 (10)
O4	0.0384 (12)	0.0528 (14)	0.0187 (9)	0.0059 (10)	0.0006 (8)	-0.0108 (9)
C5	0.0231 (12)	0.0328 (14)	0.0198 (12)	0.0011 (11)	0.0039 (10)	0.0005 (10)
C6	0.0214 (12)	0.0246 (12)	0.0184 (11)	-0.0007 (10)	0.0013 (9)	0.0013 (9)
N7	0.0208 (10)	0.0286 (11)	0.0219 (11)	-0.0005 (9)	0.0026 (8)	-0.0035 (9)
C8	0.0194 (13)	0.0424 (17)	0.0393 (16)	-0.0025 (12)	0.0046 (11)	-0.0122 (13)
C9	0.0196 (13)	0.058 (2)	0.052 (2)	-0.0004 (14)	-0.0009 (13)	-0.0263 (17)
N10	0.0228 (11)	0.0442 (15)	0.0318 (13)	0.0043 (10)	-0.0017 (9)	-0.0169 (11)
C11	0.0240 (12)	0.0289 (13)	0.0197 (12)	0.0039 (10)	0.0016 (9)	-0.0033 (10)
C12	0.0344 (17)	0.080 (3)	0.048 (2)	0.0120 (18)	-0.0026 (15)	-0.042 (2)
C15	0.0198 (13)	0.0505 (19)	0.0376 (16)	-0.0005 (12)	0.0060 (11)	-0.0174 (14)
C16	0.063 (3)	0.070 (3)	0.051 (2)	0.037 (2)	0.0086 (19)	0.004 (2)
C17	0.064 (2)	0.053 (2)	0.0292 (16)	-0.0114 (18)	0.0255 (15)	-0.0032 (15)
C18	0.129 (4)	0.0362 (19)	0.049 (2)	0.006 (2)	0.044 (3)	0.0110 (17)

Geometric parameters (Å, º)

B1—C15	1.608 (4)	C12—H12A	0.9900
B1—C17	1.610 (5)	C12—H12B	0.9900
B1—C11	1.618 (4)	C12—H12C	0.9900
B1—N1	1.623 (3)	C12—H12D	0.9900

N1—C6	1.364 (3)	C13—O14	1.409 (5)
N1—C2	1.365 (3)	C13—H13A	0.9900
C2—O2	1.227 (3)	C13—H13B	0.9900
C2—N3	1.382 (3)	O14—H14	0.8400
N3—C4	1.383 (4)	C13A—O14A	1.432 (6)
N3—H3	0.880 (18)	C13A—H13C	0.9900
C4—O4	1.233 (3)	C13A—H13D	0.9900
C4—C5	1.435 (4)	O14A—H14A	0.8400
C5—C6	1.346 (4)	C15—C16	1.516 (6)
C5—H5	0.9500	C15—H15A	0.9900
C6—N7	1.408 (3)	C15—H15B	0.9900
N7—C11	1.353 (3)	C16—H16A	0.9800
N7—C8	1.388 (3)	C16—H16B	0.9800
C8—C9	1.343 (4)	C16—H16C	0.9800
C8—H8	0.9500	C17—C18	1.497 (6)
C9—N10	1.396 (4)	C17—H17A	0.9900
C9—H9	0.9500	C17—H17B	0.9900
N10—C11	1.326 (3)	C18—H18A	0.9800
N10—C12	1.477 (4)	C18—H18B	0.9800
C12—C13A	1.536 (5)	C18—H18C	0.9800
C12—C13	1.573 (5)		
C15—B1—C17	114.9 (3)	H12A—C12—H12B	108.0
C15—B1—C11	114.8 (2)	N10—C12—H12C	108.7
C17—B1—C11	110.8 (3)	C13A—C12—H12C	108.7
C15—B1—N1	111.6 (2)	N10—C12—H12D	108.7
C17—B1—N1	110.1 (2)	C13A—C12—H12D	108.7
C11—B1—N1	92.37 (19)	H12C—C12—H12D	107.6
C6—N1—C2	119.0 (2)	O14—C13—C12	108.4 (4)
C6—N1—B1	115.2 (2)	O14—C13—H13A	110.0
C2—N1—B1	125.8 (2)	C12—C13—H13A	110.0
O2—C2—N1	122.6 (2)	O14—C13—H13B	110.0
O2—C2—N3	121.5 (3)	C12—C13—H13B	110.0
N1—C2—N3	115.9 (2)	H13A—C13—H13B	108.4
C2—N3—C4	126.8 (2)	C13—O14—H14	109.5
C2—N3—H3	116 (2)	O14A—C13A—C12	98.1 (5)
C4—N3—H3	117 (2)	O14A—C13A—H13C	112.1
O4—C4—N3	120.0 (3)	C12—C13A—H13C	112.1
O4—C4—C5	125.1 (3)	O14A—C13A—H13D	112.1

N3—C4—C5	114.9 (2)	C12—C13A—H13D	112.1
C6—C5—C4	117.0 (2)	H13C—C13A—H13D	109.8
C6—C5—H5	121.5	C13A—O14A—H14A	109.5
C4—C5—H5	121.5	C16—C15—B1	116.7 (3)
C5—C6—N1	126.1 (2)	C16—C15—H15A	108.1
C5—C6—N7	126.8 (2)	B1—C15—H15A	108.1
N1—C6—N7	107.1 (2)	C16—C15—H15B	108.1
C11—N7—C8	111.0 (2)	B1—C15—H15B	108.1
C11—N7—C6	113.0 (2)	H15A—C15—H15B	107.3
C8—N7—C6	136.0 (2)	C15—C16—H16A	109.5
C9—C8—N7	105.1 (3)	C15—C16—H16B	109.5
C9—C8—H8	127.5	H16A—C16—H16B	109.5
N7—C8—H8	127.5	C15—C16—H16C	109.5
C8—C9—N10	108.3 (3)	H16A—C16—H16C	109.5
C8—C9—H9	125.8	H16B—C16—H16C	109.5
N10—C9—H9	125.8	C18—C17—B1	117.0 (3)
C11—N10—C9	109.4 (2)	C18—C17—H17A	108.0
C11—N10—C12	123.3 (2)	B1—C17—H17A	108.0
C9—N10—C12	127.3 (3)	C18—C17—H17B	108.0
N10—C11—N7	106.2 (2)	B1—C17—H17B	108.0
N10—C11—B1	141.4 (2)	H17A—C17—H17B	107.3
N7—C11—B1	112.2 (2)	C17—C18—H18A	109.5
N10—C12—C13A	114.4 (4)	C17—C18—H18B	109.5
N10—C12—C13	111.7 (3)	H18A—C18—H18B	109.5
N10—C12—H12A	109.3	C17—C18—H18C	109.5
C13—C12—H12A	109.3	H18A—C18—H18C	109.5
N10—C12—H12B	109.3	H18B—C18—H18C	109.5
C13—C12—H12B	109.3		
C15—B1—N1—C6	-118.9 (3)	C8—C9—N10—C12	179.6 (3)
C17—B1—N1—C6	112.2 (3)	C9—N10—C11—N7	0.9 (4)
C11—B1—N1—C6	-1.0 (3)	C12—N10—C11—N7	-178.9 (3)
C15—B1—N1—C2	65.4 (4)	C9—N10—C11—B1	-172.9 (4)
C17—B1—N1—C2	-63.5 (4)	C12—N10—C11—B1	7.2 (6)
C11—B1—N1—C2	-176.7 (3)	C8—N7—C11—N10	-1.3 (3)
C6—N1—C2—O2	-177.4 (3)	C6—N7—C11—N10	179.6 (2)
B1—N1—C2—O2	-1.9 (5)	C8—N7—C11—B1	174.5 (2)
C6—N1—C2—N3	3.2 (4)	C6—N7—C11—B1	-4.5 (3)
B1—N1—C2—N3	178.8 (3)	C15—B1—C11—N10	-68.1 (5)

O2—C2—N3—C4	-177.6 (3)	C17—B1—C11—N10	64.2 (5)
N1—C2—N3—C4	1.8 (5)	N1—B1—C11—N10	176.7 (4)
C2—N3—C4—O4	178.1 (3)	C15—B1—C11—N7	118.3 (3)
C2—N3—C4—C5	-3.8 (4)	C17—B1—C11—N7	-109.4 (3)
O4—C4—C5—C6	178.7 (3)	N1—B1—C11—N7	3.1 (3)
N3—C4—C5—C6	0.8 (4)	C11—N10—C12—C13A	-144.4 (4)
C4—C5—C6—N1	4.3 (4)	C9—N10—C12—C13A	35.7 (6)
C4—C5—C6—N7	-177.1 (3)	C11—N10—C12—C13	-89.9 (4)
C2—N1—C6—C5	-6.5 (4)	C9—N10—C12—C13	90.3 (5)
B1—N1—C6—C5	177.5 (3)	N10—C12—C13—O14	-61.3 (5)
C2—N1—C6—N7	174.7 (2)	C13A—C12—C13—O14	43.0 (6)
B1—N1—C6—N7	-1.3 (3)	N10—C12—C13A—O14A	78.0 (7)
C5—C6—N7—C11	-175.1 (3)	C13—C12—C13A—O14A	-20.5 (5)
N1—C6—N7—C11	3.6 (3)	C17—B1—C15—C16	179.5 (3)
C5—C6—N7—C8	6.1 (5)	C11—B1—C15—C16	-50.2 (4)
N1—C6—N7—C8	-175.1 (3)	N1—B1—C15—C16	53.3 (4)
C11—N7—C8—C9	1.1 (4)	C15—B1—C17—C18	-176.0 (3)
C6—N7—C8—C9	179.9 (3)	C11—B1—C17—C18	51.8 (4)
N7—C8—C9—N10	-0.5 (4)	N1—B1—C17—C18	-48.9 (4)
C8—C9—N10—C11	-0.3 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O2^{i}	0.88 (2)	1.99 (2)	2.848 (3)	166 (3)
C12—H12*A*···O14^{ii}	0.99	2.18	3.084 (7)	151
O14—H14···O4^{iii}	0.84	2.20	2.695 (5)	118
O14*A*—H14*A*···O4^{iii}	0.84	2.02	2.748 (9)	145

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

1-Benzyl-10,10-diethyl-6,8-dioxo-6,7,8,10-tetrahydro-1H-imidazo [2',1:3,4][1,4,2]diazaborolo[1,5-c]pyrimidinium-10-ide – 25d

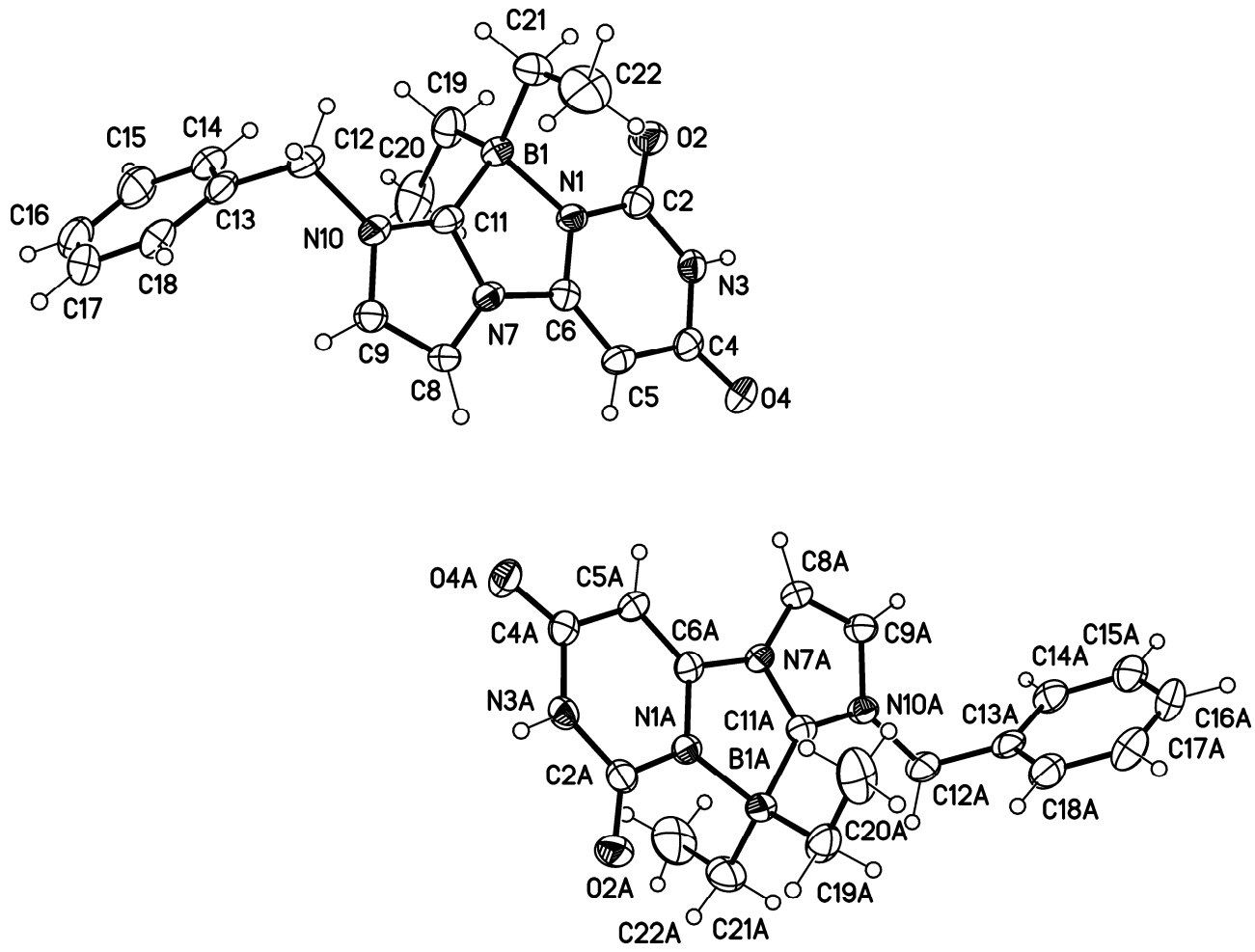


Fig. S3: Molecular structure of **25d** (displacement parameters are drawn at 50% probability level)

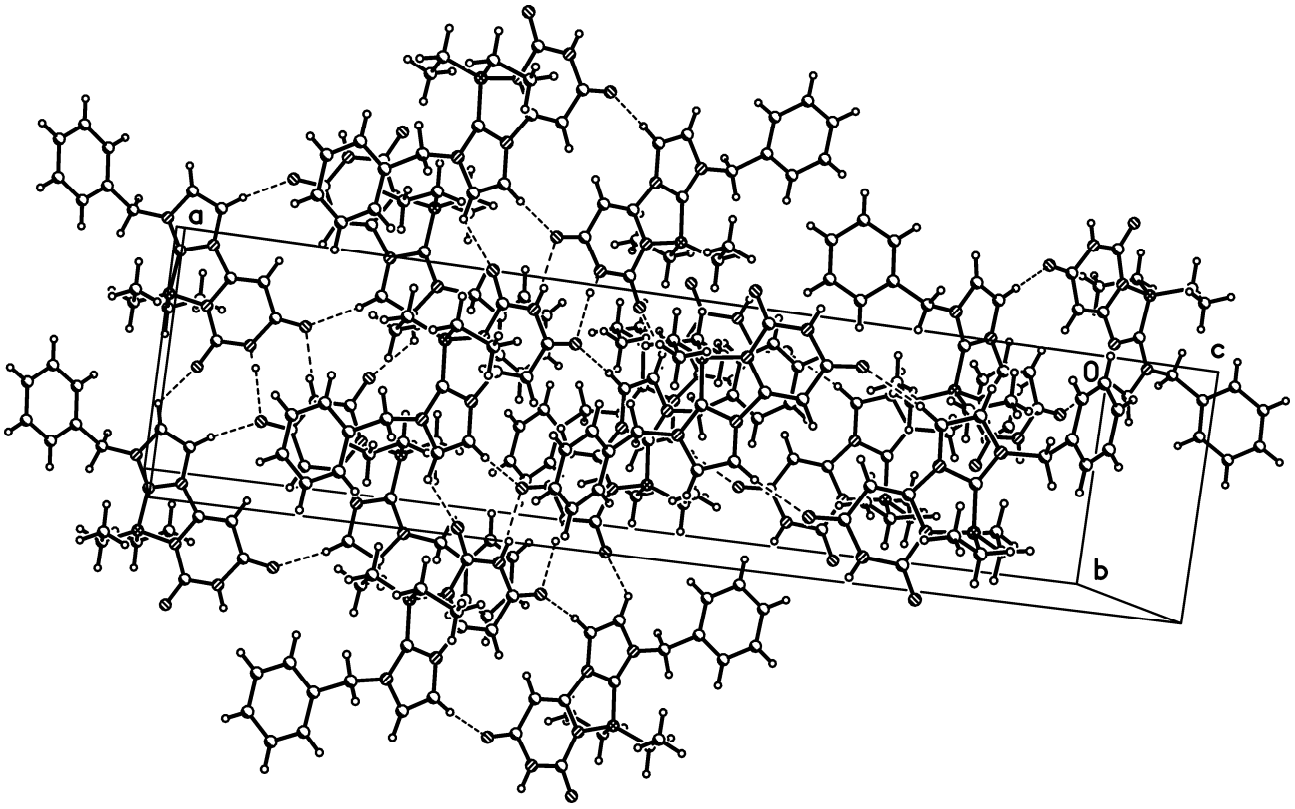


Fig. S4: Packing diagram of **25d**

1-Benzyl-10,10-diethyl-6,8-dioxo-6,7,8,10-tetrahydro-1H-imidazo [2',1:3,4][1,4,2]diazaborolo[1,5-c]pyrimidinium-10-ide – 25d

Crystal data

$C_{18}H_{21}BN_4O_2$	D_x = 1.258 Mg m^{-3}
M_r = 336.20	Mo $K\alpha$ radiation, λ = 0.71073 Å
Orthorhombic, $Pna2_1$ (no.33)	Cell parameters from 182 reflections
a = 35.612 (3) Å	θ = 2.5–25.0°
b = 8.829 (1) Å	μ = 0.08 mm^{-1}
c = 11.287 (1) Å	T = 123 K
V = 3548.8 (6) Å^3	Blocks, colourless
Z = 8	0.40 × 0.30 × 0.20 mm
F(000) = 1424	

Data collection

Bruker-Nonius KappaCCD diffractometer	6456 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.033
rotation in ϕ and ω, 0.5° scans	θ_{max} = 27.5°, θ_{min} = 2.6°
Absorption correction: multi-scan *SADABS* (Sheldrick, 2008)	h = -46→45
T_{min} = 0.935, T_{max} = 0.987	k = -11→10
22454 measured reflections	l = -14→14
7540 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.117	$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.8778P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.12	$(\Delta/\sigma)_{max} < 0.001$
7540 reflections	$\Delta\rangle_{max}$ = 0.31 e Å^{-3}
457 parameters	$\Delta\rangle_{min}$ = -0.22 e Å^{-3}
3 restraints	Absolute structure: Flack x determined using 2474 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons and Flack (2004), Acta Cryst. A60, s61).
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: -0.7 (5)

Computing details

Data collection: Collect; cell refinement: *EVALCCD*; data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXS97*; program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2013); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *publCIF*.

Special details

Experimental. dx = 60 mm, 140 sec./deg., 0.5 deg., 3 sets, 898 frames, 10883 refl. postref.
Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
B1	0.74525 (9)	0.2835 (4)	0.8398 (3)	0.0239 (7)
N1	0.70667 (7)	0.2569 (3)	0.7652 (2)	0.0244 (6)
C2	0.69154 (9)	0.1194 (3)	0.7366 (3)	0.0281 (7)
O2	0.70596 (7)	-0.0007 (3)	0.7614 (2)	0.0419 (6)
N3	0.65788 (7)	0.1253 (3)	0.6749 (2)	0.0271 (6)
H3	0.6500 (9)	0.039 (3)	0.649 (3)	0.032*
C4	0.63853 (9)	0.2531 (4)	0.6402 (3)	0.0269 (7)
O4	0.60861 (6)	0.2405 (3)	0.5846 (2)	0.0329 (5)
C5	0.65578 (8)	0.3934 (4)	0.6732 (3)	0.0262 (6)
H5	0.6447	0.4881	0.6542	0.031*
C6	0.68851 (8)	0.3846 (3)	0.7325 (3)	0.0233 (6)
N7	0.71001 (6)	0.5080 (3)	0.7714 (2)	0.0238 (5)
C8	0.70692 (8)	0.6629 (3)	0.7652 (3)	0.0244 (6)
H8	0.6876	0.7198	0.7278	0.029*
C9	0.73710 (8)	0.7171 (3)	0.8233 (3)	0.0252 (6)
H9	0.7432	0.8207	0.8347	0.030*
N10	0.75766 (6)	0.5930 (3)	0.8636 (2)	0.0243 (5)
C11	0.74127 (7)	0.4645 (3)	0.8316 (3)	0.0244 (6)
C12	0.79286 (8)	0.6039 (4)	0.9325 (3)	0.0301 (7)
H12A	0.8007	0.5012	0.9576	0.036*
H12B	0.7884	0.6650	1.0046	0.036*
C13	0.82389 (8)	0.6759 (4)	0.8601 (3)	0.0295 (7)
C14	0.84797 (8)	0.5856 (4)	0.7948 (3)	0.0350 (8)
H14	0.8454	0.4785	0.7970	0.042*

C15	0.87587 (9)	0.6508 (5)	0.7262 (4)	0.0437 (9)
H15	0.8926	0.5882	0.6826	0.052*
C16	0.87942 (10)	0.8058 (5)	0.7211 (4)	0.0457 (10)
H16	0.8983	0.8501	0.6730	0.055*
C17	0.85545 (9)	0.8973 (4)	0.7860 (4)	0.0411 (9)
H17	0.8578	1.0043	0.7822	0.049*
C18	0.82802 (9)	0.8316 (4)	0.8565 (3)	0.0343 (8)
H18	0.8120	0.8940	0.9027	0.041*
C19	0.78100 (9)	0.2183 (4)	0.7689 (3)	0.0359 (8)
H19A	0.8039	0.2409	0.8155	0.043*
H19B	0.7786	0.1067	0.7643	0.043*
C20	0.78661 (11)	0.2793 (6)	0.6435 (4)	0.0534 (11)
H20A	0.8091	0.2333	0.6085	0.080*
H20B	0.7897	0.3896	0.6464	0.080*
H20C	0.7646	0.2543	0.5950	0.080*
C21	0.74115 (10)	0.2207 (4)	0.9735 (3)	0.0367 (8)
H21A	0.7398	0.1088	0.9705	0.044*
H21B	0.7642	0.2479	1.0180	0.044*
C22	0.70753 (12)	0.2785 (6)	1.0418 (4)	0.0583 (12)
H22A	0.7076	0.2348	1.1216	0.087*
H22B	0.6844	0.2489	1.0006	0.087*
H22C	0.7088	0.3891	1.0473	0.087*
B1A	0.50278 (10)	0.7793 (4)	0.3247 (3)	0.0261 (7)
N1A	0.54180 (7)	0.8068 (3)	0.3939 (2)	0.0228 (5)
C2A	0.55577 (9)	0.9456 (3)	0.4267 (3)	0.0276 (7)
O2A	0.54006 (6)	1.0635 (3)	0.4033 (2)	0.0385 (6)
N3A	0.58910 (7)	0.9433 (3)	0.4898 (2)	0.0263 (6)
H3A	0.5974 (9)	1.032 (3)	0.511 (3)	0.032*
C4A	0.61050 (8)	0.8173 (3)	0.5171 (3)	0.0249 (7)
O4A	0.64058 (6)	0.8335 (3)	0.5706 (2)	0.0329 (5)
C5A	0.59455 (8)	0.6762 (3)	0.4812 (3)	0.0237 (6)
H5A	0.6069	0.5829	0.4970	0.028*
C6A	0.56148 (8)	0.6806 (3)	0.4242 (3)	0.0224 (6)
N7A	0.54031 (6)	0.5557 (3)	0.3859 (2)	0.0219 (5)
C8A	0.54333 (8)	0.4003 (3)	0.3939 (3)	0.0254 (6)
H8A	0.5630	0.3440	0.4297	0.031*
C9A	0.51248 (8)	0.3453 (3)	0.3400 (3)	0.0273 (6)
H9A	0.5063	0.2414	0.3301	0.033*
N10A	0.49131 (6)	0.4687 (3)	0.3013 (2)	0.0252 (5)

C11A	0.50814 (8)	0.5971 (3)	0.3298 (2)	0.0229 (6)
C12A	0.45551 (9)	0.4571 (4)	0.2366 (3)	0.0308 (7)
H12C	0.4599	0.4050	0.1601	0.037*
H12D	0.4460	0.5601	0.2192	0.037*
C13A	0.42635 (8)	0.3715 (4)	0.3060 (3)	0.0291 (7)
C14A	0.42243 (9)	0.2165 (4)	0.2920 (3)	0.0321 (7)
H14A	0.4379	0.1640	0.2372	0.039*
C15A	0.39573 (9)	0.1372 (4)	0.3581 (4)	0.0429 (9)
H15A	0.3933	0.0306	0.3494	0.051*
C16A	0.37310 (9)	0.2142 (5)	0.4356 (4)	0.0477 (10)
H16A	0.3546	0.1608	0.4796	0.057*
C17A	0.37690 (9)	0.3672 (5)	0.4504 (4)	0.0488 (10)
H17A	0.3612	0.4192	0.5050	0.059*
C18A	0.40337 (9)	0.4463 (4)	0.3863 (4)	0.0399 (8)
H18A	0.4059	0.5525	0.3972	0.048*
C19A	0.46770 (9)	0.8319 (4)	0.4039 (4)	0.0401 (9)
H19C	0.4671	0.9440	0.4052	0.048*
H19D	0.4444	0.7969	0.3648	0.048*
C20A	0.46753 (12)	0.7751 (5)	0.5313 (4)	0.0503 (10)
H20D	0.4452	0.8137	0.5722	0.075*
H20E	0.4902	0.8108	0.5720	0.075*
H20F	0.4671	0.6641	0.5316	0.075*
C21A	0.50425 (11)	0.8440 (4)	0.1923 (3)	0.0423 (9)
H21C	0.4807	0.8149	0.1515	0.051*
H21D	0.5048	0.9560	0.1964	0.051*
C22A	0.53684 (14)	0.7920 (6)	0.1178 (4)	0.0581 (12)
H22D	0.5351	0.8376	0.0388	0.087*
H22E	0.5363	0.6814	0.1106	0.087*
H22F	0.5604	0.8231	0.1553	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0227 (15)	0.0253 (16)	0.0238 (17)	0.0030 (13)	-0.0017 (14)	-0.0014 (14)
N1	0.0218 (12)	0.0271 (15)	0.0242 (14)	0.0025 (9)	0.0005 (11)	0.0033 (11)
C2	0.0262 (15)	0.0300 (18)	0.0281 (17)	-0.0005 (13)	0.0007 (13)	-0.0003 (14)
O2	0.0397 (13)	0.0306 (13)	0.0555 (17)	0.0030 (10)	-0.0127 (12)	0.0029 (12)
N3	0.0251 (13)	0.0250 (14)	0.0311 (14)	-0.0045 (10)	-0.0004 (11)	-0.0001 (11)
C4	0.0205 (15)	0.0367 (19)	0.0235 (16)	0.0003 (12)	0.0047 (12)	0.0007 (13)

O4	0.0226 (11)	0.0395 (13)	0.0365 (13)	-0.0020 (9)	-0.0050 (10)	-0.0037 (10)
C5	0.0225 (14)	0.0306 (17)	0.0253 (15)	0.0060 (12)	-0.0006 (12)	0.0007 (13)
C6	0.0243 (14)	0.0265 (16)	0.0191 (14)	-0.0005 (11)	0.0027 (12)	-0.0017 (12)
N7	0.0200 (11)	0.0290 (14)	0.0224 (13)	0.0022 (10)	-0.0013 (10)	0.0013 (11)
C8	0.0238 (13)	0.0239 (14)	0.0254 (15)	0.0022 (11)	-0.0019 (12)	0.0045 (12)
C9	0.0265 (14)	0.0235 (14)	0.0256 (15)	0.0008 (11)	-0.0024 (13)	0.0005 (12)
N10	0.0218 (11)	0.0285 (13)	0.0225 (12)	0.0007 (10)	-0.0031 (10)	-0.0007 (10)
C11	0.0205 (13)	0.0335 (16)	0.0190 (14)	0.0039 (11)	0.0002 (11)	0.0027 (12)
C12	0.0271 (15)	0.0375 (18)	0.0257 (16)	0.0013 (13)	-0.0071 (13)	0.0002 (14)
C13	0.0222 (14)	0.0395 (18)	0.0269 (17)	-0.0019 (13)	-0.0082 (13)	0.0006 (14)
C14	0.0220 (14)	0.0379 (18)	0.045 (2)	0.0033 (13)	-0.0053 (14)	0.0050 (16)
C15	0.0250 (17)	0.051 (2)	0.055 (2)	0.0042 (15)	0.0027 (16)	0.001 (2)
C16	0.0244 (17)	0.065 (3)	0.048 (2)	-0.0084 (16)	-0.0041 (16)	0.009 (2)
C17	0.0360 (17)	0.0378 (19)	0.049 (2)	-0.0108 (15)	-0.0122 (17)	0.0028 (17)
C18	0.0276 (16)	0.0426 (19)	0.0326 (18)	-0.0029 (14)	-0.0091 (14)	-0.0062 (15)
C19	0.0259 (15)	0.0322 (16)	0.049 (2)	0.0027 (12)	0.0035 (15)	-0.0066 (16)
C20	0.037 (2)	0.084 (3)	0.039 (2)	-0.0107 (19)	0.0148 (17)	-0.020 (2)
C21	0.0407 (18)	0.0368 (19)	0.0325 (18)	-0.0021 (15)	-0.0074 (15)	0.0100 (15)
C22	0.059 (3)	0.090 (3)	0.026 (2)	0.001 (2)	0.0141 (18)	0.011 (2)
B1A	0.0245 (16)	0.0246 (16)	0.0291 (19)	-0.0001 (13)	-0.0049 (15)	0.0032 (15)
N1A	0.0220 (12)	0.0236 (14)	0.0228 (13)	0.0007 (9)	-0.0002 (11)	0.0004 (10)
C2A	0.0282 (15)	0.0244 (16)	0.0302 (17)	-0.0026 (12)	0.0023 (13)	0.0028 (13)
O2A	0.0372 (12)	0.0221 (12)	0.0561 (16)	0.0021 (9)	-0.0107 (12)	0.0034 (11)
N3A	0.0280 (13)	0.0183 (13)	0.0326 (14)	-0.0032 (10)	0.0000 (11)	-0.0014 (11)
C4A	0.0227 (15)	0.0289 (17)	0.0231 (15)	-0.0006 (12)	0.0033 (13)	-0.0012 (12)
O4A	0.0234 (11)	0.0355 (13)	0.0397 (13)	-0.0022 (9)	-0.0051 (10)	-0.0043 (11)
C5A	0.0197 (14)	0.0271 (16)	0.0244 (15)	0.0037 (11)	-0.0003 (12)	-0.0011 (13)
C6A	0.0208 (14)	0.0260 (16)	0.0206 (15)	0.0014 (11)	0.0052 (12)	-0.0012 (12)
N7A	0.0193 (11)	0.0233 (13)	0.0231 (12)	0.0022 (9)	-0.0001 (10)	-0.0019 (10)
C8A	0.0232 (13)	0.0261 (16)	0.0270 (15)	0.0041 (11)	-0.0018 (12)	0.0005 (13)
C9A	0.0298 (15)	0.0228 (14)	0.0294 (16)	0.0023 (12)	-0.0063 (13)	-0.0004 (13)
N10A	0.0244 (12)	0.0256 (12)	0.0256 (13)	0.0015 (10)	-0.0034 (10)	0.0007 (11)
C11A	0.0242 (13)	0.0255 (14)	0.0190 (14)	0.0016 (11)	0.0010 (11)	0.0006 (12)
C12A	0.0307 (16)	0.0355 (18)	0.0263 (16)	-0.0015 (13)	-0.0123 (13)	0.0011 (13)
C13A	0.0238 (14)	0.0310 (17)	0.0326 (17)	0.0021 (12)	-0.0129 (13)	0.0007 (13)
C14A	0.0292 (16)	0.0359 (17)	0.0314 (19)	-0.0007 (13)	-0.0103 (15)	-0.0051 (14)
C15A	0.0327 (17)	0.0385 (19)	0.057 (2)	-0.0087 (14)	-0.0151 (17)	0.0037 (17)
C16A	0.0219 (18)	0.060 (3)	0.061 (3)	-0.0074 (16)	-0.0004 (18)	0.009 (2)
C17A	0.0248 (17)	0.060 (3)	0.062 (3)	0.0071 (16)	0.0051 (17)	0.001 (2)

C18A	0.0285 (16)	0.0383 (19)	0.053 (2)	0.0037 (13)	-0.0037 (16)	0.0012 (17)
C19A	0.0263 (15)	0.0279 (17)	0.066 (3)	0.0026 (12)	0.0003 (16)	-0.0067 (17)
C20A	0.050 (2)	0.049 (2)	0.052 (3)	-0.0062 (18)	0.027 (2)	-0.0140 (19)
C21A	0.050 (2)	0.042 (2)	0.0352 (19)	-0.0061 (17)	-0.0139 (17)	0.0115 (17)
C22A	0.071 (3)	0.076 (3)	0.028 (2)	-0.012 (2)	0.006 (2)	0.011 (2)

Geometric parameters (Å, º)

B1—C11	1.607 (5)	B1A—C21A	1.601 (5)
B1—C19	1.610 (5)	B1A—C19A	1.604 (5)
B1—C21	1.615 (5)	B1A—N1A	1.612 (4)
B1—N1	1.628 (4)	B1A—C11A	1.622 (5)
N1—C6	1.351 (4)	N1A—C6A	1.360 (4)
N1—C2	1.367 (4)	N1A—C2A	1.374 (4)
C2—O2	1.211 (4)	C2A—O2A	1.211 (4)
C2—N3	1.388 (4)	C2A—N3A	1.384 (4)
N3—C4	1.379 (4)	N3A—C4A	1.383 (4)
N3—H3	0.86 (2)	N3A—H3A	0.87 (2)
C4—O4	1.242 (4)	C4A—O4A	1.238 (4)
C4—C5	1.432 (5)	C4A—C5A	1.428 (4)
C5—C6	1.346 (4)	C5A—C6A	1.343 (4)
C5—H5	0.9500	C5A—H5A	0.9500
C6—N7	1.402 (4)	C6A—N7A	1.404 (4)
N7—C11	1.359 (4)	N7A—C11A	1.359 (4)
N7—C8	1.374 (4)	N7A—C8A	1.379 (4)
C8—C9	1.347 (4)	C8A—C9A	1.346 (4)
C8—H8	0.9500	C8A—H8A	0.9500
C9—N10	1.394 (4)	C9A—N10A	1.395 (4)
C9—H9	0.9500	C9A—H9A	0.9500
N10—C11	1.327 (4)	N10A—C11A	1.321 (4)
N10—C12	1.478 (3)	N10A—C12A	1.473 (4)
C12—C13	1.514 (4)	C12A—C13A	1.504 (5)
C12—H12A	0.9900	C12A—H12C	0.9900
C12—H12B	0.9900	C12A—H12D	0.9900
C13—C18	1.383 (5)	C13A—C14A	1.385 (5)
C13—C14	1.384 (5)	C13A—C18A	1.388 (5)
C14—C15	1.385 (5)	C14A—C15A	1.397 (5)
C14—H14	0.9500	C14A—H14A	0.9500
C15—C16	1.376 (6)	C15A—C16A	1.370 (6)

C15—H15	0.9500	C15A—H15A	0.9500
C16—C17	1.385 (6)	C16A—C17A	1.369 (6)
C16—H16	0.9500	C16A—H16A	0.9500
C17—C18	1.387 (5)	C17A—C18A	1.378 (5)
C17—H17	0.9500	C17A—H17A	0.9500
C18—H18	0.9500	C18A—H18A	0.9500
C19—C20	1.528 (6)	C19A—C20A	1.523 (6)
C19—H19A	0.9900	C19A—H19C	0.9900
C19—H19B	0.9900	C19A—H19D	0.9900
C20—H20A	0.9800	C20A—H20D	0.9800
C20—H20B	0.9800	C20A—H20E	0.9800
C20—H20C	0.9800	C20A—H20F	0.9800
C21—C22	1.512 (5)	C21A—C22A	1.505 (6)
C21—H21A	0.9900	C21A—H21C	0.9900
C21—H21B	0.9900	C21A—H21D	0.9900
C22—H22A	0.9800	C22A—H22D	0.9800
C22—H22B	0.9800	C22A—H22E	0.9800
C22—H22C	0.9800	C22A—H22F	0.9800
C11—B1—C19	113.4 (3)	C21A—B1A—C19A	116.2 (3)
C11—B1—C21	112.8 (3)	C21A—B1A—N1A	111.7 (3)
C19—B1—C21	114.4 (3)	C19A—B1A—N1A	111.0 (3)
C11—B1—N1	92.2 (2)	C21A—B1A—C11A	112.5 (3)
C19—B1—N1	111.0 (3)	C19A—B1A—C11A	111.1 (3)
C21—B1—N1	110.9 (2)	N1A—B1A—C11A	91.8 (2)
C6—N1—C2	119.2 (3)	C6A—N1A—C2A	118.5 (3)
C6—N1—B1	115.1 (2)	C6A—N1A—B1A	116.3 (2)
C2—N1—B1	125.6 (2)	C2A—N1A—B1A	125.2 (2)
O2—C2—N1	123.8 (3)	O2A—C2A—N1A	122.7 (3)
O2—C2—N3	121.0 (3)	O2A—C2A—N3A	121.4 (3)
N1—C2—N3	115.2 (3)	N1A—C2A—N3A	115.9 (3)
C4—N3—C2	127.3 (3)	C4A—N3A—C2A	126.8 (3)
C4—N3—H3	118 (2)	C4A—N3A—H3A	119 (2)
C2—N3—H3	115 (2)	C2A—N3A—H3A	115 (2)
O4—C4—N3	119.9 (3)	O4A—C4A—N3A	119.5 (3)
O4—C4—C5	125.3 (3)	O4A—C4A—C5A	125.7 (3)
N3—C4—C5	114.8 (3)	N3A—C4A—C5A	114.8 (3)
C6—C5—C4	116.8 (3)	C6A—C5A—C4A	117.4 (3)
C6—C5—H5	121.6	C6A—C5A—H5A	121.3

C4—C5—H5	121.6	C4A—C5A—H5A	121.3
C5—C6—N1	126.8 (3)	C5A—C6A—N1A	126.6 (3)
C5—C6—N7	125.7 (3)	C5A—C6A—N7A	126.6 (3)
N1—C6—N7	107.5 (2)	N1A—C6A—N7A	106.8 (3)
C11—N7—C8	111.9 (2)	C11A—N7A—C8A	111.3 (2)
C11—N7—C6	112.6 (2)	C11A—N7A—C6A	112.7 (2)
C8—N7—C6	135.5 (2)	C8A—N7A—C6A	136.0 (2)
C9—C8—N7	105.3 (3)	C9A—C8A—N7A	105.4 (3)
C9—C8—H8	127.3	C9A—C8A—H8A	127.3
N7—C8—H8	127.3	N7A—C8A—H8A	127.3
C8—C9—N10	107.4 (3)	C8A—C9A—N10A	107.5 (3)
C8—C9—H9	126.3	C8A—C9A—H9A	126.3
N10—C9—H9	126.3	N10A—C9A—H9A	126.3
C11—N10—C9	110.6 (2)	C11A—N10A—C9A	110.4 (2)
C11—N10—C12	124.9 (2)	C11A—N10A—C12A	125.0 (2)
C9—N10—C12	124.5 (2)	C9A—N10A—C12A	124.6 (2)
N10—C11—N7	104.8 (2)	N10A—C11A—N7A	105.4 (2)
N10—C11—B1	142.8 (3)	N10A—C11A—B1A	142.1 (3)
N7—C11—B1	112.5 (2)	N7A—C11A—B1A	112.5 (2)
N10—C12—C13	111.2 (2)	N10A—C12A—C13A	112.0 (2)
N10—C12—H12A	109.4	N10A—C12A—H12C	109.2
C13—C12—H12A	109.4	C13A—C12A—H12C	109.2
N10—C12—H12B	109.4	N10A—C12A—H12D	109.2
C13—C12—H12B	109.4	C13A—C12A—H12D	109.2
H12A—C12—H12B	108.0	H12C—C12A—H12D	107.9
C18—C13—C14	119.4 (3)	C14A—C13A—C18A	119.0 (3)
C18—C13—C12	120.7 (3)	C14A—C13A—C12A	120.4 (3)
C14—C13—C12	119.9 (3)	C18A—C13A—C12A	120.5 (3)
C13—C14—C15	120.2 (3)	C13A—C14A—C15A	120.2 (3)
C13—C14—H14	119.9	C13A—C14A—H14A	119.9
C15—C14—H14	119.9	C15A—C14A—H14A	119.9
C16—C15—C14	120.2 (3)	C16A—C15A—C14A	119.6 (4)
C16—C15—H15	119.9	C16A—C15A—H15A	120.2
C14—C15—H15	119.9	C14A—C15A—H15A	120.2
C15—C16—C17	120.1 (3)	C17A—C16A—C15A	120.6 (4)
C15—C16—H16	120.0	C17A—C16A—H16A	119.7
C17—C16—H16	120.0	C15A—C16A—H16A	119.7
C16—C17—C18	119.6 (3)	C16A—C17A—C18A	120.3 (4)
C16—C17—H17	120.2	C16A—C17A—H17A	119.8

C18—C17—H17	120.2	C18A—C17A—H17A	119.8
C13—C18—C17	120.5 (3)	C17A—C18A—C13A	120.3 (4)
C13—C18—H18	119.8	C17A—C18A—H18A	119.8
C17—C18—H18	119.8	C13A—C18A—H18A	119.8
C20—C19—B1	115.9 (3)	C20A—C19A—B1A	115.7 (3)
C20—C19—H19A	108.3	C20A—C19A—H19C	108.4
B1—C19—H19A	108.3	B1A—C19A—H19C	108.4
C20—C19—H19B	108.3	C20A—C19A—H19D	108.4
B1—C19—H19B	108.3	B1A—C19A—H19D	108.4
H19A—C19—H19B	107.4	H19C—C19A—H19D	107.4
C19—C20—H20A	109.5	C19A—C20A—H20D	109.5
C19—C20—H20B	109.5	C19A—C20A—H20E	109.5
H20A—C20—H20B	109.5	H20D—C20A—H20E	109.5
C19—C20—H20C	109.5	C19A—C20A—H20F	109.5
H20A—C20—H20C	109.5	H20D—C20A—H20F	109.5
H20B—C20—H20C	109.5	H20E—C20A—H20F	109.5
C22—C21—B1	115.6 (3)	C22A—C21A—B1A	116.0 (3)
C22—C21—H21A	108.4	C22A—C21A—H21C	108.3
B1—C21—H21A	108.4	B1A—C21A—H21C	108.3
C22—C21—H21B	108.4	C22A—C21A—H21D	108.3
B1—C21—H21B	108.4	B1A—C21A—H21D	108.3
H21A—C21—H21B	107.4	H21C—C21A—H21D	107.4
C21—C22—H22A	109.5	C21A—C22A—H22D	109.5
C21—C22—H22B	109.5	C21A—C22A—H22E	109.5
H22A—C22—H22B	109.5	H22D—C22A—H22E	109.5
C21—C22—H22C	109.5	C21A—C22A—H22F	109.5
H22A—C22—H22C	109.5	H22D—C22A—H22F	109.5
H22B—C22—H22C	109.5	H22E—C22A—H22F	109.5
C11—B1—N1—C6	-1.2 (3)	C21A—B1A—N1A—C6A	-114.6 (3)
C19—B1—N1—C6	-117.4 (3)	C19A—B1A—N1A—C6A	113.9 (3)
C21—B1—N1—C6	114.2 (3)	C11A—B1A—N1A—C6A	0.5 (3)
C11—B1—N1—C2	-179.9 (3)	C21A—B1A—N1A—C2A	67.4 (4)
C19—B1—N1—C2	64.0 (4)	C19A—B1A—N1A—C2A	-64.1 (4)
C21—B1—N1—C2	-64.4 (4)	C11A—B1A—N1A—C2A	-177.5 (3)
C6—N1—C2—O2	179.4 (3)	C6A—N1A—C2A—O2A	180.0 (3)
B1—N1—C2—O2	-2.0 (5)	B1A—N1A—C2A—O2A	-2.0 (5)
C6—N1—C2—N3	-0.1 (4)	C6A—N1A—C2A—N3A	-0.5 (4)
B1—N1—C2—N3	178.5 (3)	B1A—N1A—C2A—N3A	177.4 (3)

O2—C2—N3—C4	-179.5 (3)	O2A—C2A—N3A—C4A	-176.8 (3)
N1—C2—N3—C4	0.0 (4)	N1A—C2A—N3A—C4A	3.7 (4)
C2—N3—C4—O4	179.7 (3)	C2A—N3A—C4A—O4A	177.2 (3)
C2—N3—C4—C5	-0.2 (4)	C2A—N3A—C4A—C5A	-3.9 (4)
O4—C4—C5—C6	-179.4 (3)	O4A—C4A—C5A—C6A	179.8 (3)
N3—C4—C5—C6	0.5 (4)	N3A—C4A—C5A—C6A	1.0 (4)
C4—C5—C6—N1	-0.7 (4)	C4A—C5A—C6A—N1A	1.9 (4)
C4—C5—C6—N7	179.2 (3)	C4A—C5A—C6A—N7A	-177.1 (3)
C2—N1—C6—C5	0.5 (5)	C2A—N1A—C6A—C5A	-2.2 (4)
B1—N1—C6—C5	-178.2 (3)	B1A—N1A—C6A—C5A	179.6 (3)
C2—N1—C6—N7	-179.4 (2)	C2A—N1A—C6A—N7A	177.0 (2)
B1—N1—C6—N7	1.8 (3)	B1A—N1A—C6A—N7A	-1.2 (3)
C5—C6—N7—C11	178.4 (3)	C5A—C6A—N7A—C11A	-179.5 (3)
N1—C6—N7—C11	-1.6 (3)	N1A—C6A—N7A—C11A	1.3 (3)
C5—C6—N7—C8	-0.4 (5)	C5A—C6A—N7A—C8A	2.9 (5)
N1—C6—N7—C8	179.6 (3)	N1A—C6A—N7A—C8A	-176.3 (3)
C11—N7—C8—C9	-0.1 (3)	C11A—N7A—C8A—C9A	0.8 (3)
C6—N7—C8—C9	178.7 (3)	C6A—N7A—C8A—C9A	178.4 (3)
N7—C8—C9—N10	-0.2 (3)	N7A—C8A—C9A—N10A	-0.4 (3)
C8—C9—N10—C11	0.4 (3)	C8A—C9A—N10A—C11A	0.0 (4)
C8—C9—N10—C12	-179.6 (3)	C8A—C9A—N10A—C12A	179.2 (3)
C9—N10—C11—N7	-0.4 (3)	C9A—N10A—C11A—N7A	0.5 (3)
C12—N10—C11—N7	179.6 (3)	C12A—N10A—C11A—N7A	-178.8 (3)
C9—N10—C11—B1	-179.8 (4)	C9A—N10A—C11A—B1A	-176.5 (4)
C12—N10—C11—B1	0.2 (6)	C12A—N10A—C11A—B1A	4.3 (6)
C8—N7—C11—N10	0.3 (3)	C8A—N7A—C11A—N10A	-0.8 (3)
C6—N7—C11—N10	-178.7 (2)	C6A—N7A—C11A—N10A	-179.0 (2)
C8—N7—C11—B1	179.9 (2)	C8A—N7A—C11A—B1A	177.2 (2)
C6—N7—C11—B1	0.8 (3)	C6A—N7A—C11A—B1A	-1.0 (3)
C19—B1—C11—N10	-66.4 (5)	C21A—B1A—C11A—N10A	-68.5 (5)
C21—B1—C11—N10	65.7 (5)	C19A—B1A—C11A—N10A	63.8 (5)
N1—B1—C11—N10	179.5 (4)	N1A—B1A—C11A—N10A	177.1 (4)
C19—B1—C11—N7	114.3 (3)	C21A—B1A—C11A—N7A	114.7 (3)
C21—B1—C11—N7	-113.7 (3)	C19A—B1A—C11A—N7A	-113.0 (3)
N1—B1—C11—N7	0.2 (3)	N1A—B1A—C11A—N7A	0.3 (3)
C11—N10—C12—C13	115.3 (3)	C11A—N10A—C12A—C13A	-122.0 (3)

C9—N10—C12—C13	-64.7 (4)	C9A—N10A—C12A—C13A	58.8 (4)
N10—C12—C13—C18	86.7 (4)	N10A—C12A—C13A—C14A	-91.7 (3)
N10—C12—C13—C14	-92.0 (3)	N10A—C12A—C13A—C18A	87.3 (4)
C18—C13—C14—C15	-0.2 (5)	C18A—C13A—C14A—C15A	-0.2 (5)
C12—C13—C14—C15	178.5 (3)	C12A—C13A—C14A—C15A	178.9 (3)
C13—C14—C15—C16	-1.0 (5)	C13A—C14A—C15A—C16A	1.0 (5)
C14—C15—C16—C17	1.0 (6)	C14A—C15A—C16A—C17A	-1.2 (6)
C15—C16—C17—C18	0.3 (6)	C15A—C16A—C17A—C18A	0.6 (6)
C14—C13—C18—C17	1.5 (5)	C16A—C17A—C18A—C13A	0.2 (6)
C12—C13—C18—C17	-177.2 (3)	C14A—C13A—C18A—C17A	-0.4 (5)
C16—C17—C18—C13	-1.6 (5)	C12A—C13A—C18A—C17A	-179.5 (3)
C11—B1—C19—C20	-46.6 (4)	C21A—B1A—C19A—C20A	-177.5 (3)
C21—B1—C19—C20	-177.9 (3)	N1A—B1A—C19A—C20A	-48.3 (4)
N1—B1—C19—C20	55.6 (4)	C11A—B1A—C19A—C20A	52.2 (4)
C11—B1—C21—C22	49.2 (4)	C19A—B1A—C21A—C22A	-178.9 (3)
C19—B1—C21—C22	-179.2 (3)	N1A—B1A—C21A—C22A	52.3 (4)
N1—B1—C21—C22	-52.7 (4)	C11A—B1A—C21A—C22A	-49.3 (4)

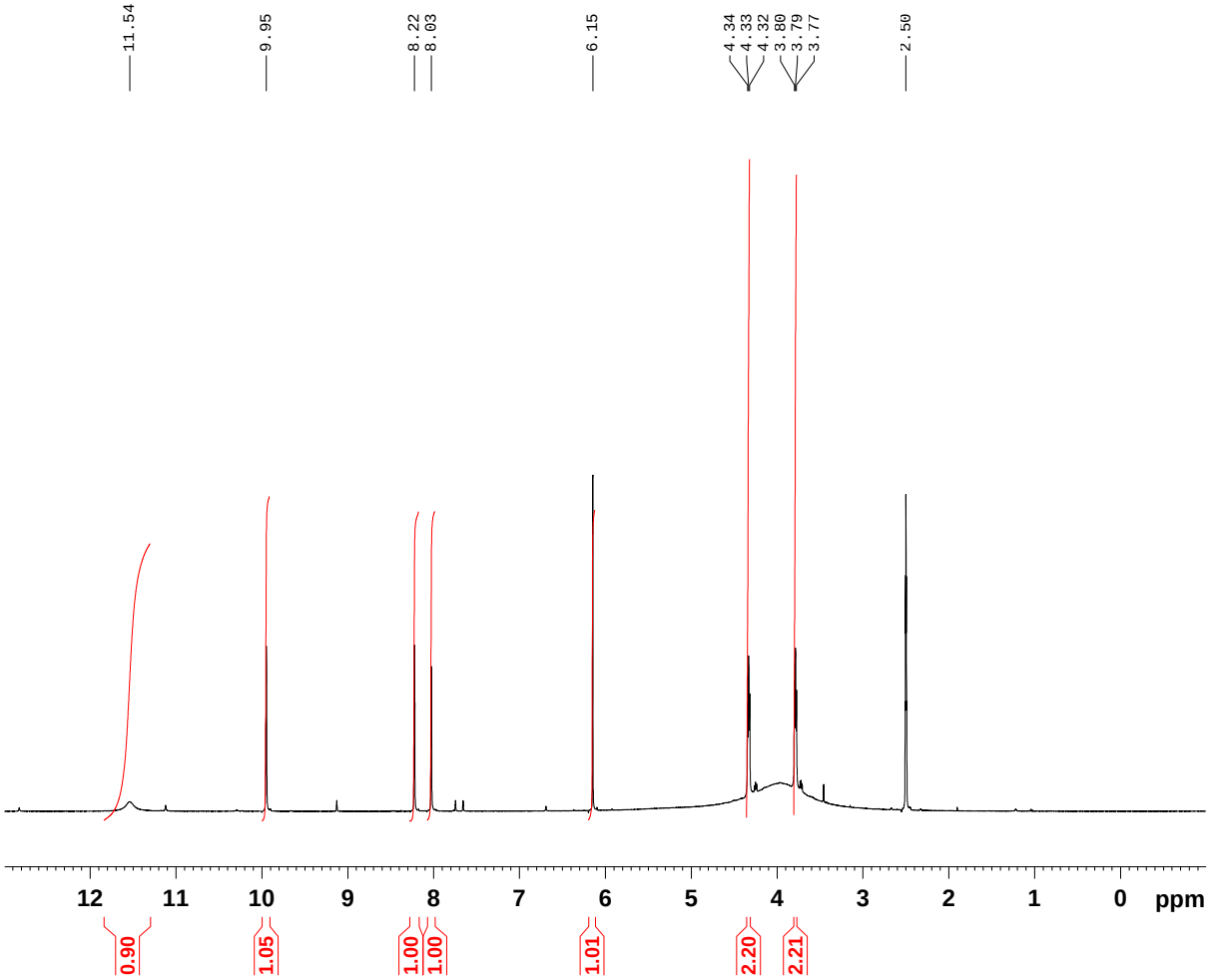
Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O4*A*^{i}	0.86 (2)	2.05 (2)	2.899 (4)	169 (3)
C8—H8···O4*A*	0.95	2.64	3.560 (4)	164
C9—H9···O2^{ii}	0.95	2.22	2.815 (4)	120
N3*A*—H3*A*···O4^{ii}	0.87 (2)	2.06 (2)	2.917 (3)	169 (3)
C8*A*—H8*A*···O4	0.95	2.55	3.469 (4)	161
C9*A*—H9*A*···O2*A*^{i}	0.95	2.14	2.769 (4)	122

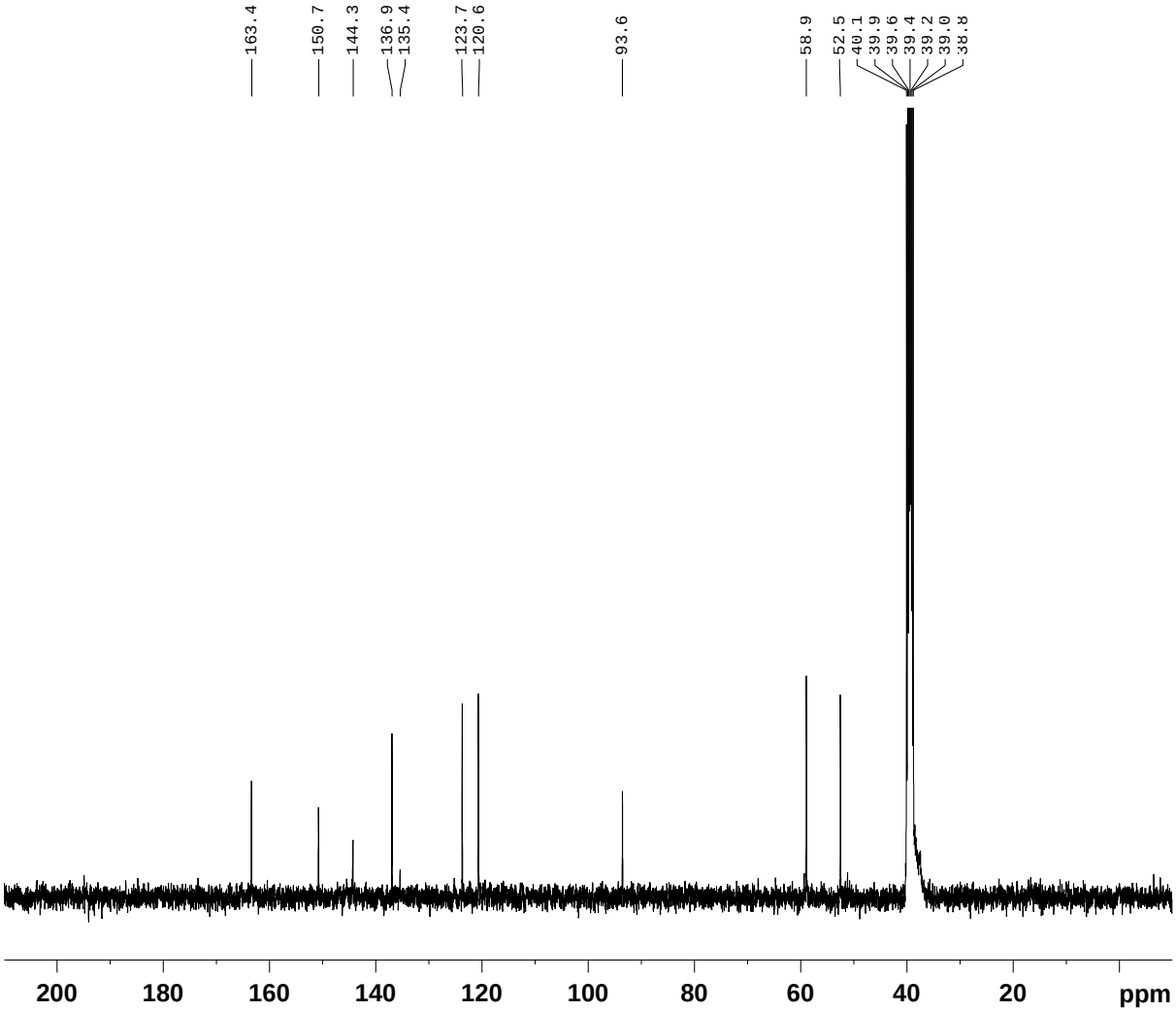
Symmetry codes: (i) *x*, *y*-1, *z*; (ii) *x*, *y*+1, *z*.

3-(2,6-Dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-1-(2-hydroxyethyl)-1*H*-imidazolium chloride 22b

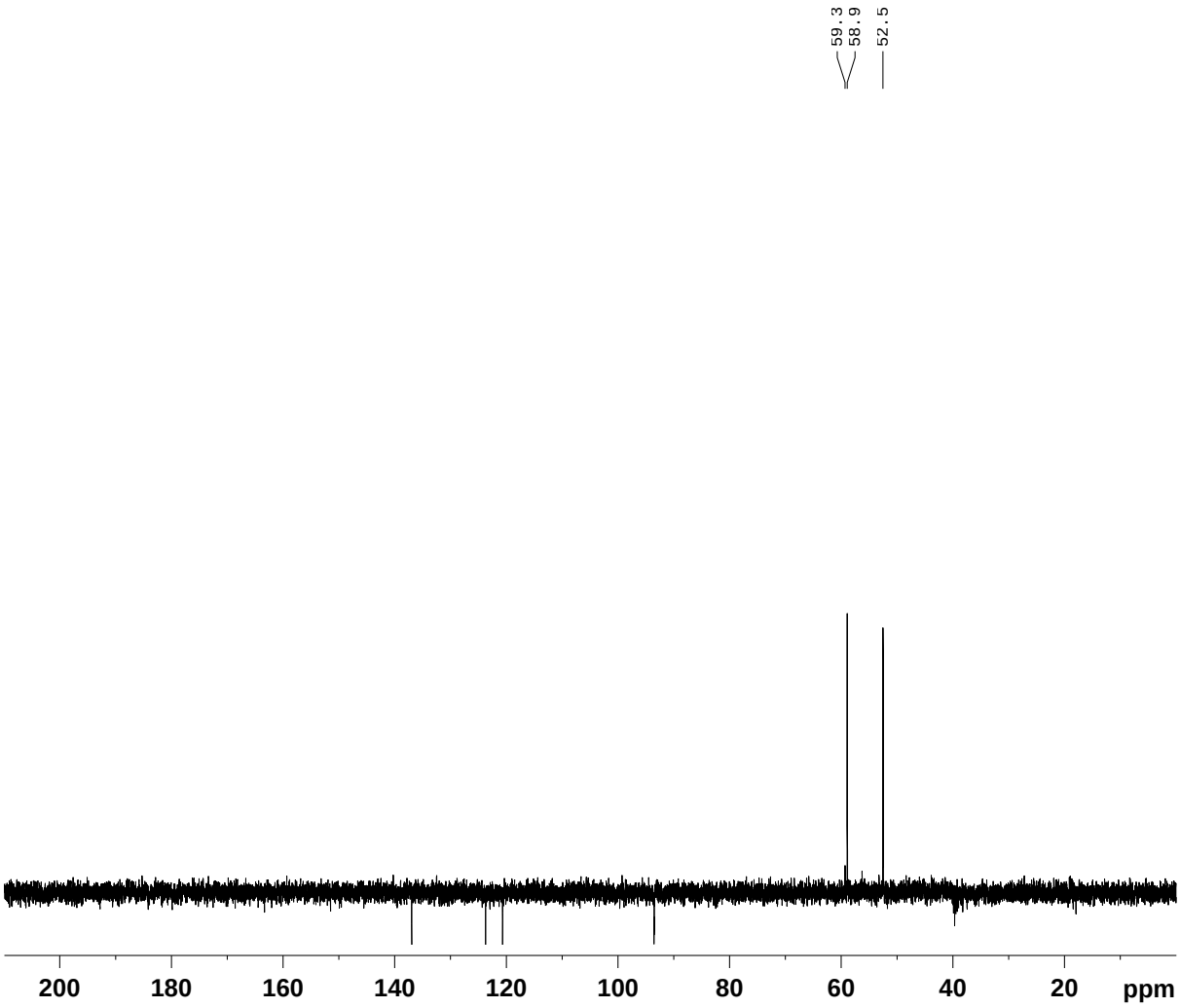
^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C NMR (100 MHz, DMSO-d_6)

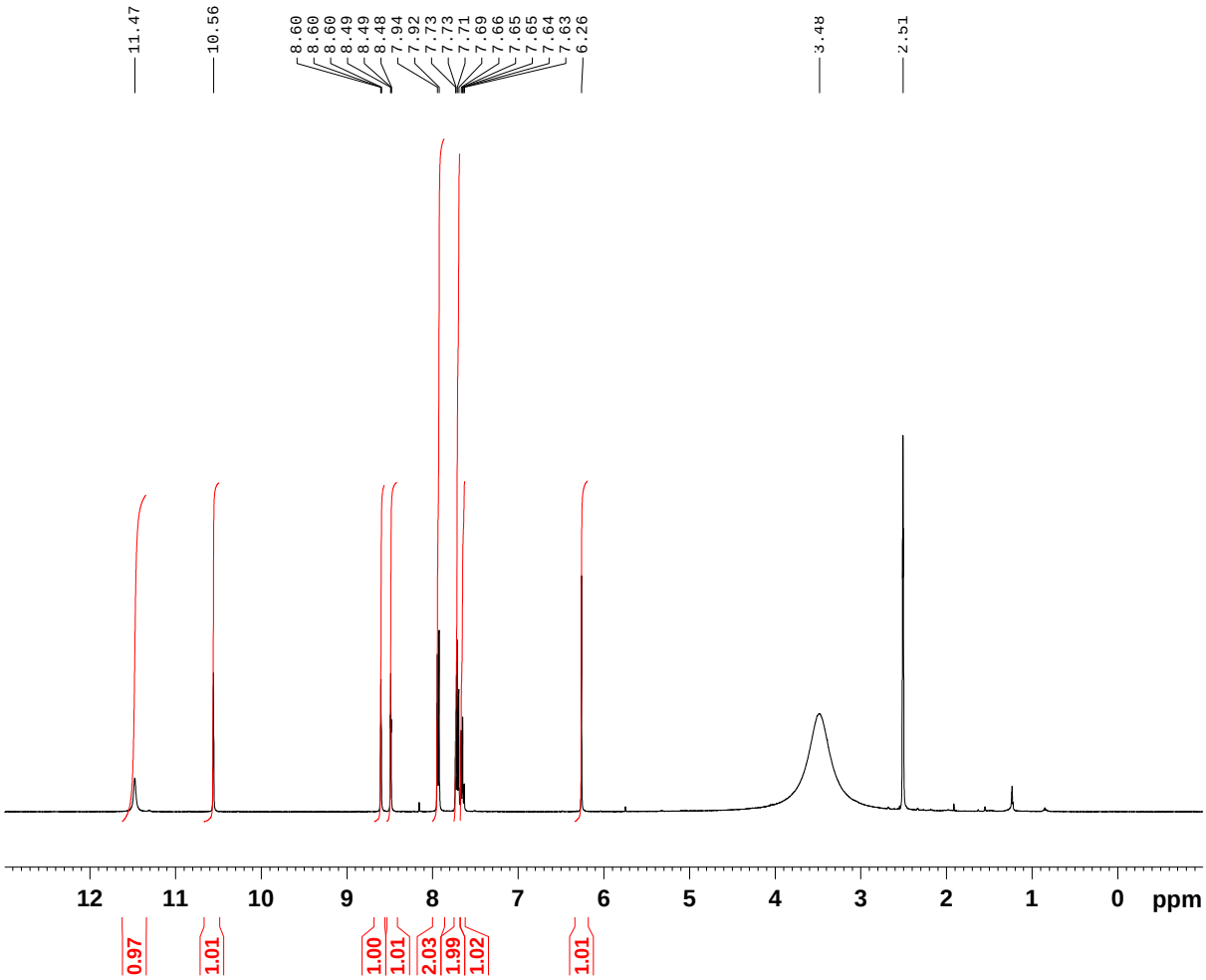


DEPT (100 MHz, DMSO-d_6)

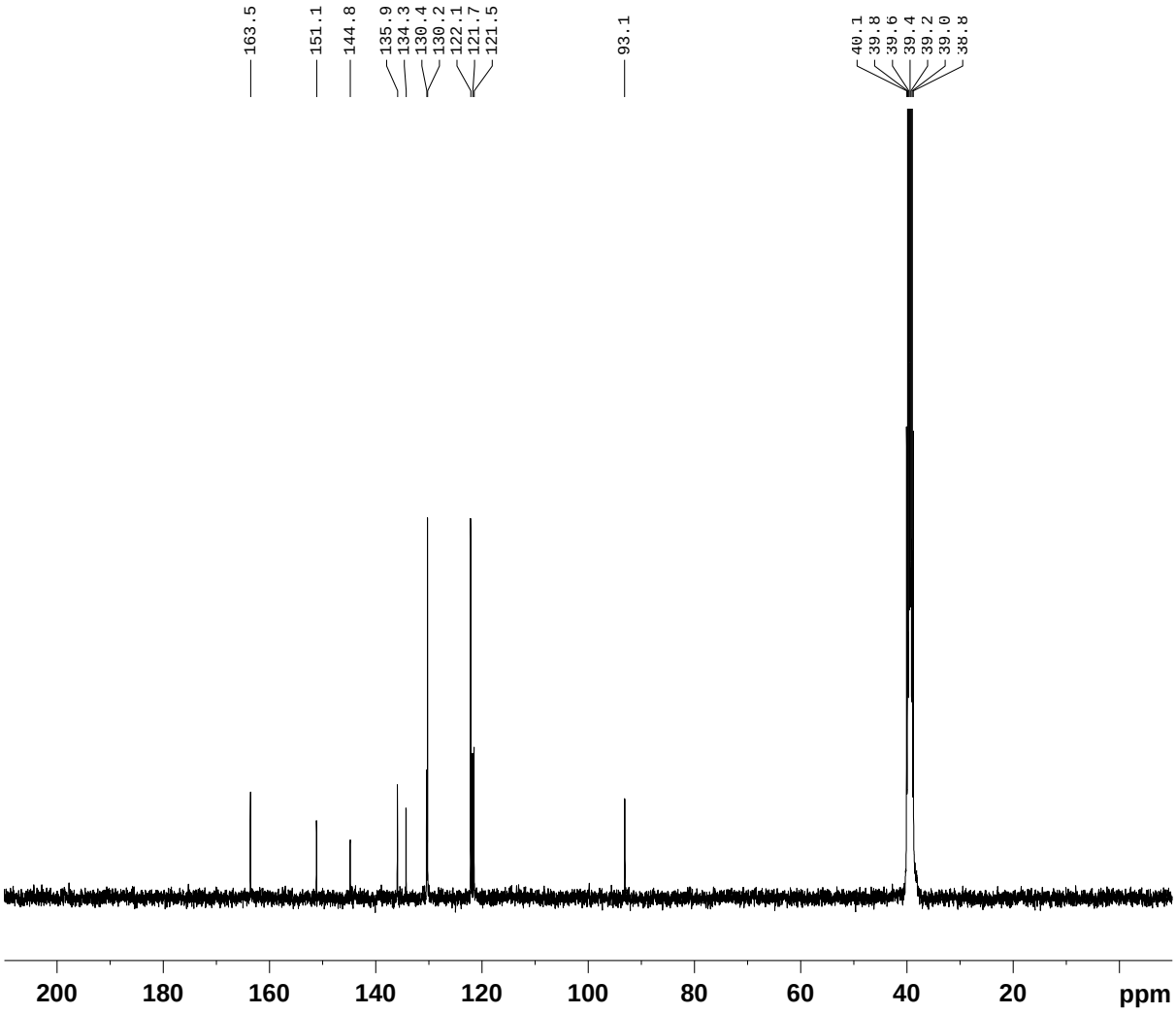


3-(2,6-Dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-1-phenyl-1*H*-imidazol-3-ium chloride 22c

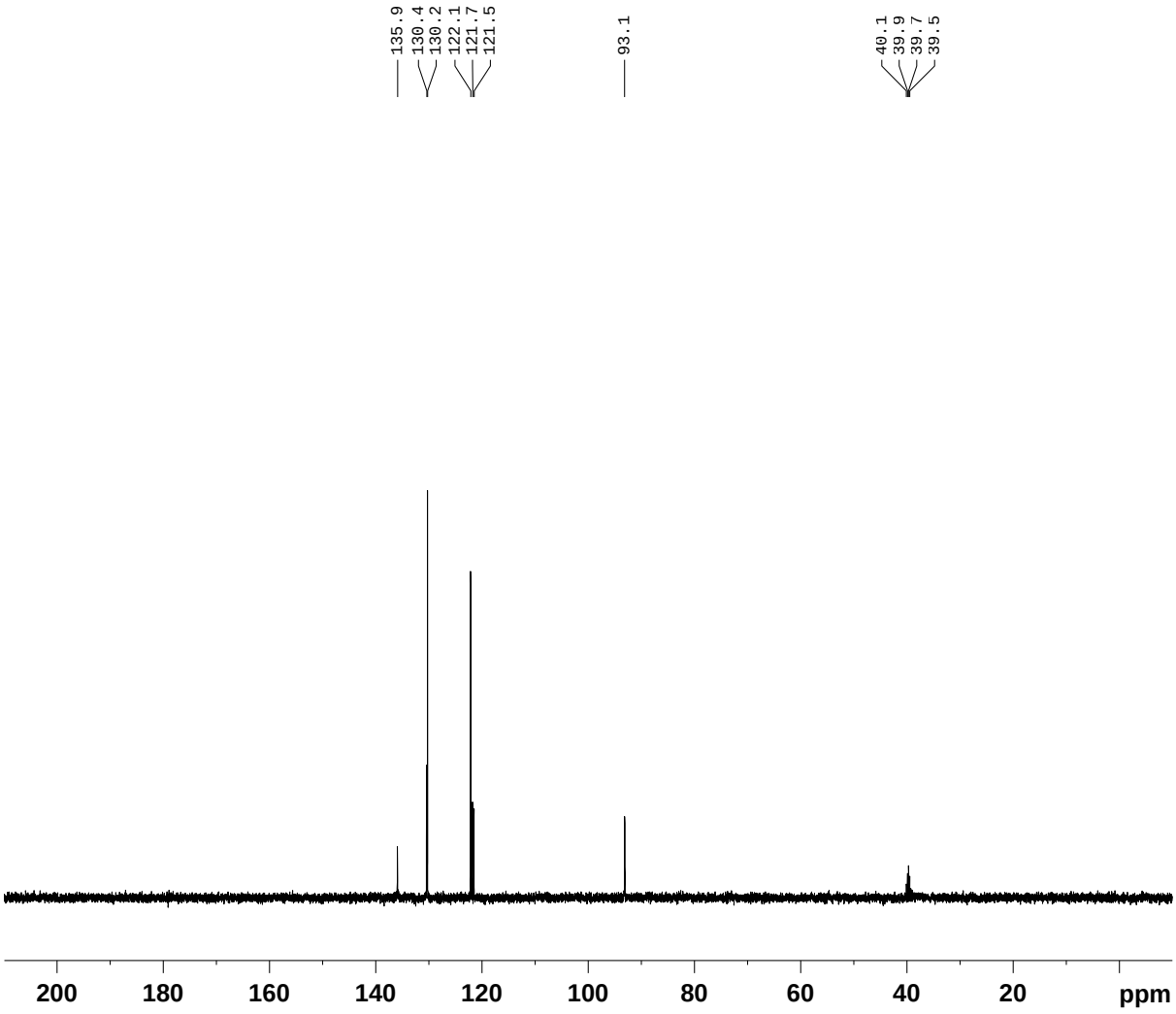
^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C NMR (100 MHz, DMSO-d_6)

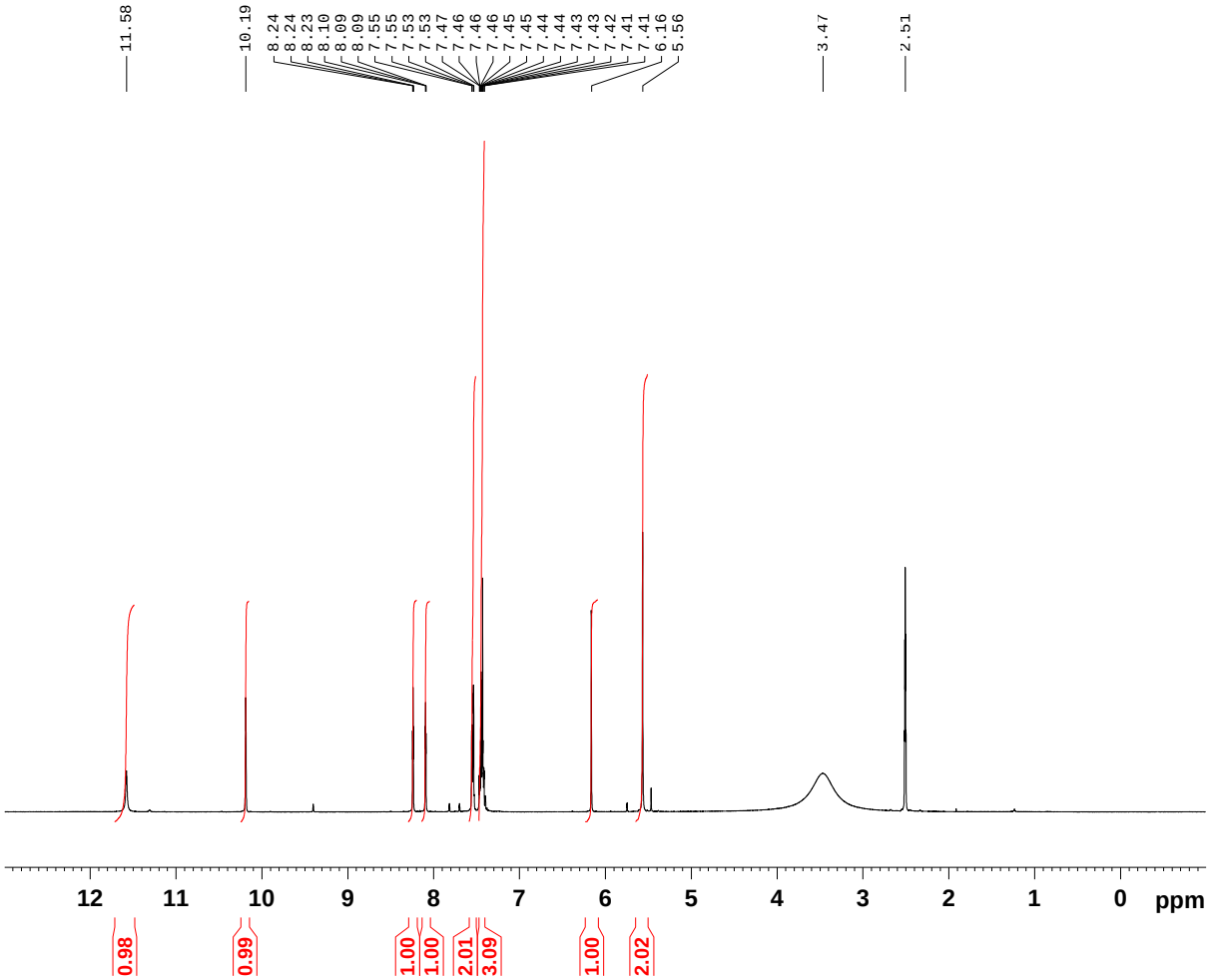


DEPT (100 MHz, DMSO-d_6)

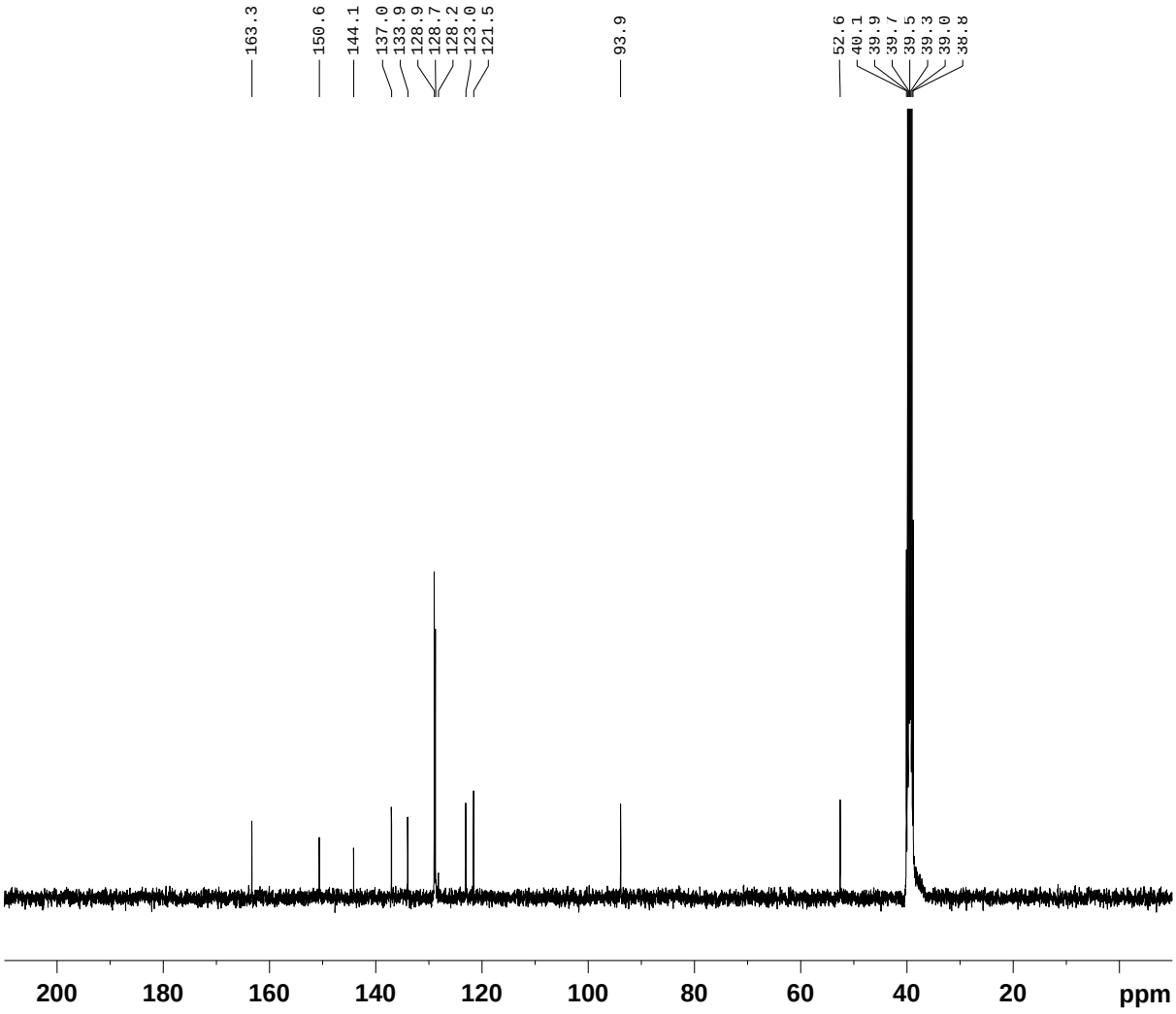


1-Benzyl-3-(2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-1*H*-imidazol-3-ium chloride 22d

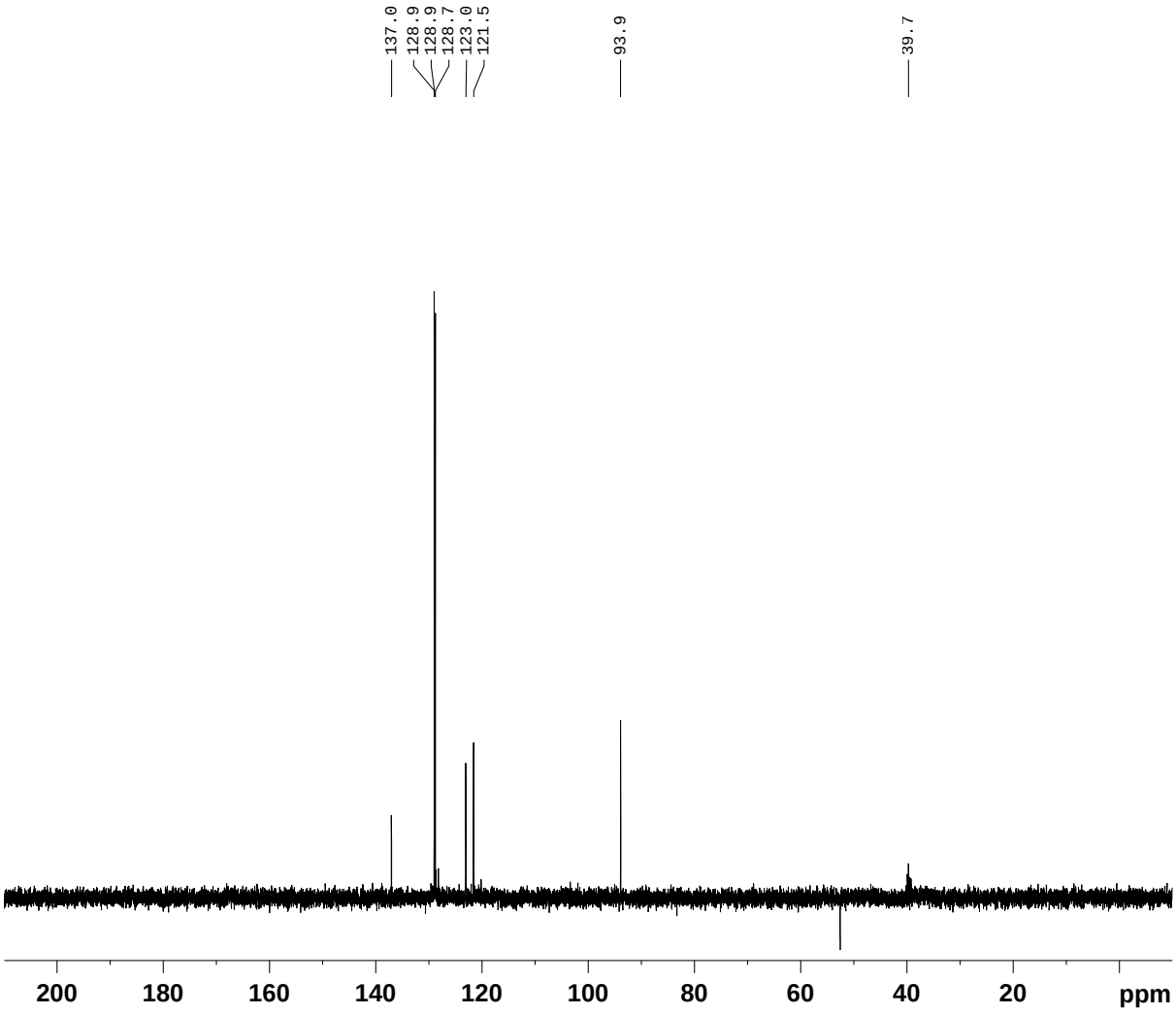
^{1}H NMR (400 MHz, DMSO-d$_6$)



^{13}C NMR (100 MHz, DMSO-d_6)

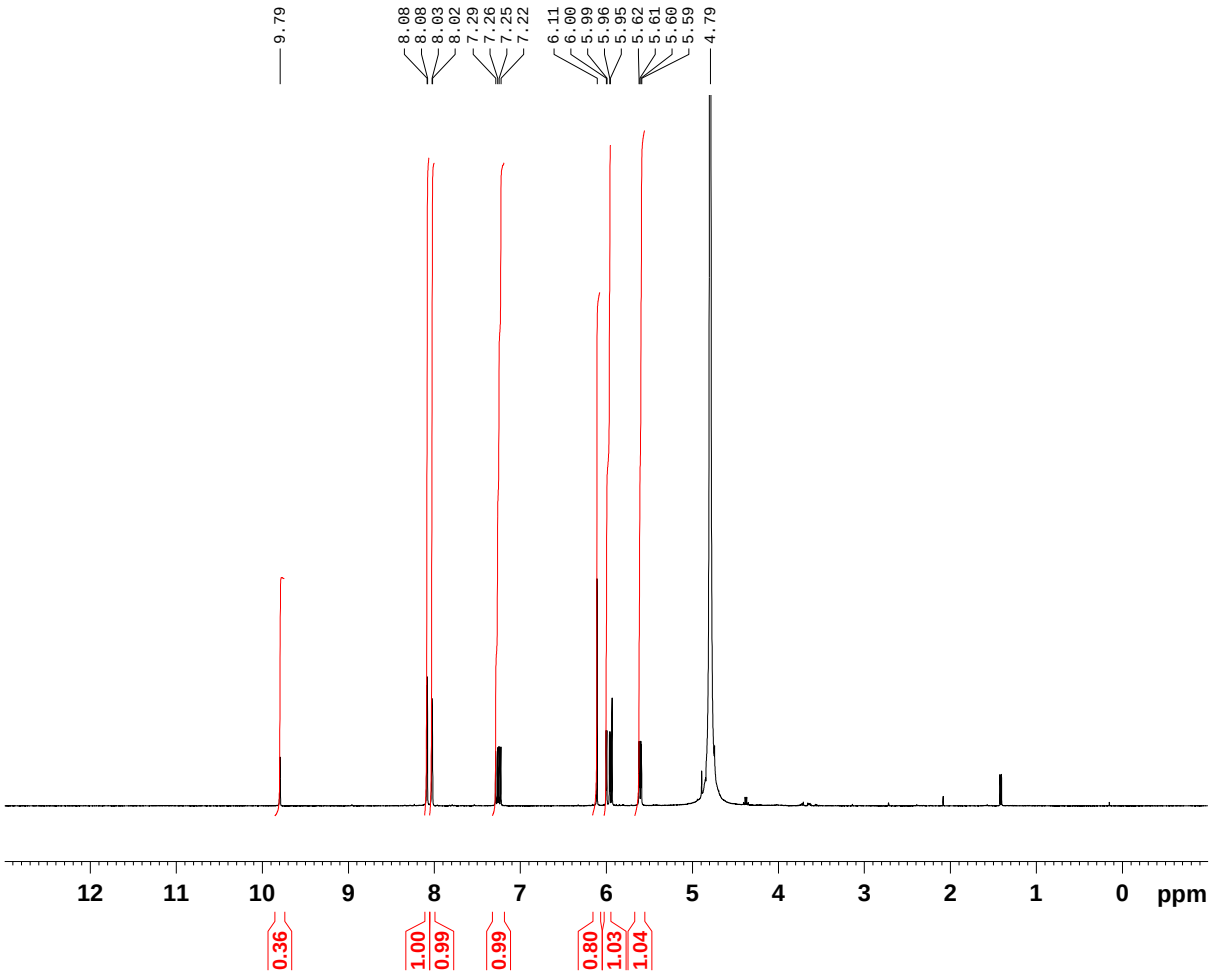


DEPT (100 MHz, DMSO-d_6)

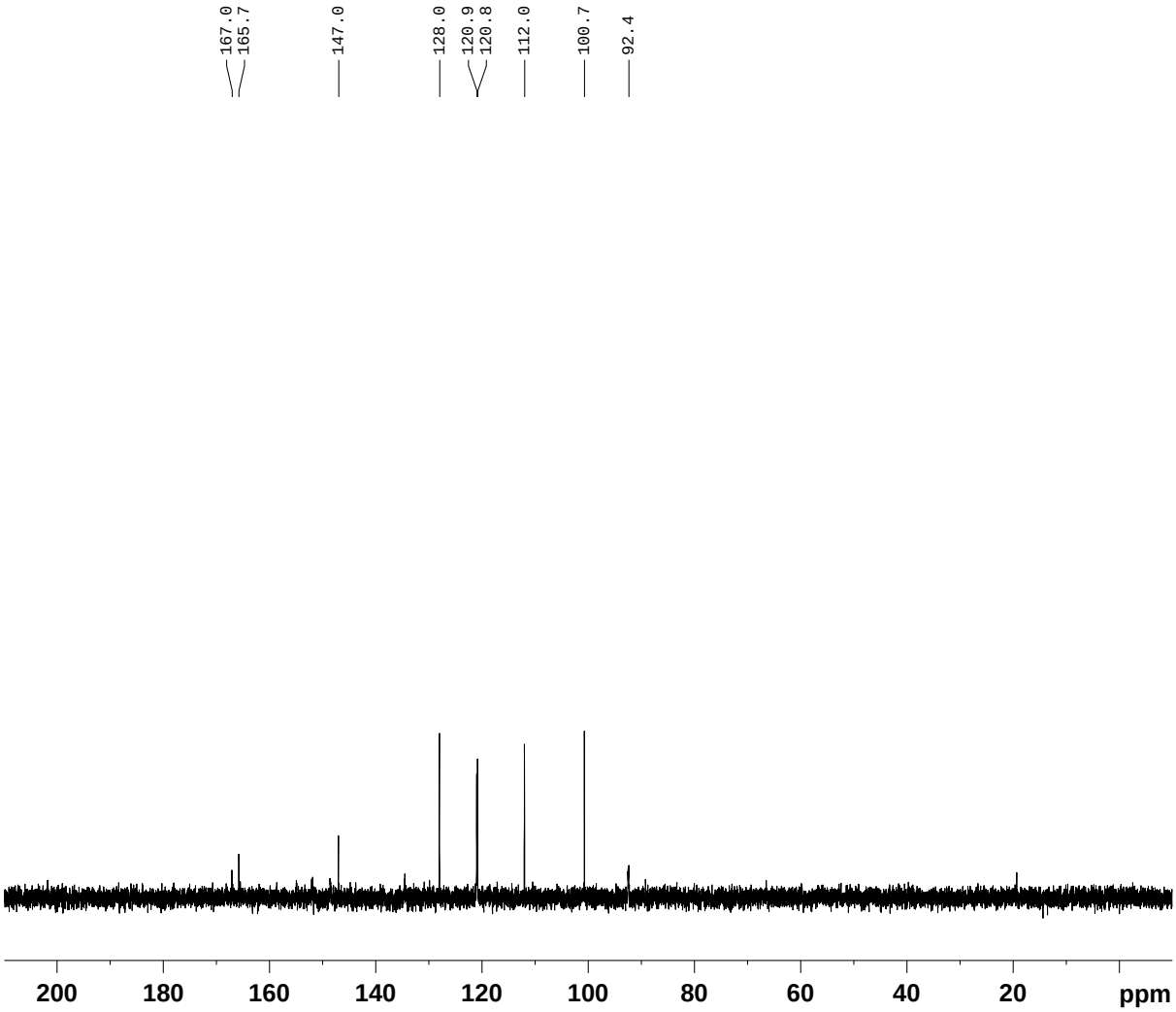


3-(2,6-Dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-1-vinyl-1*H*-imidazol-3-ium chloride 22e

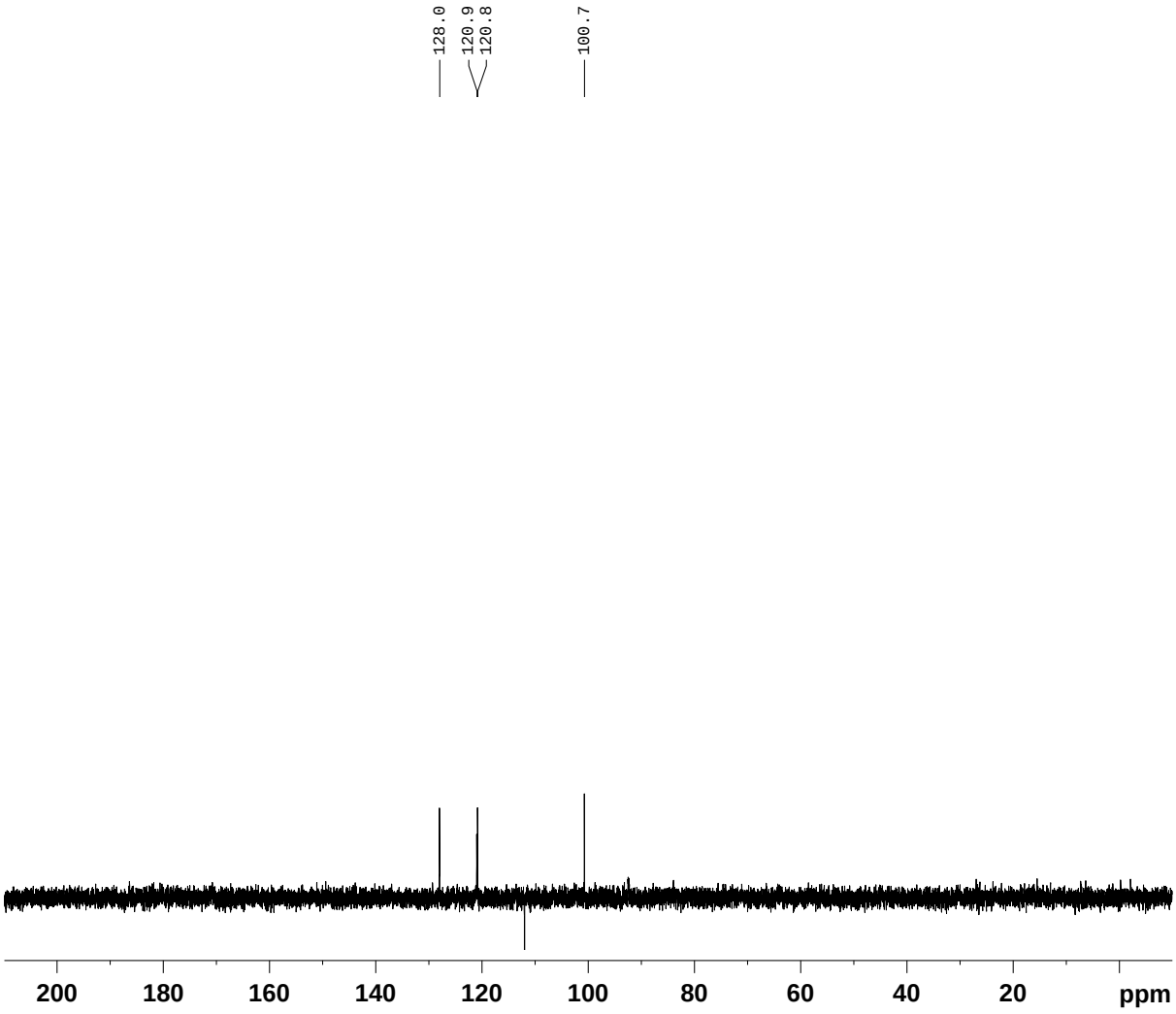
^{1}H NMR (400 MHz, D_2O)



^{13}C NMR (100 MHz, D_2O)

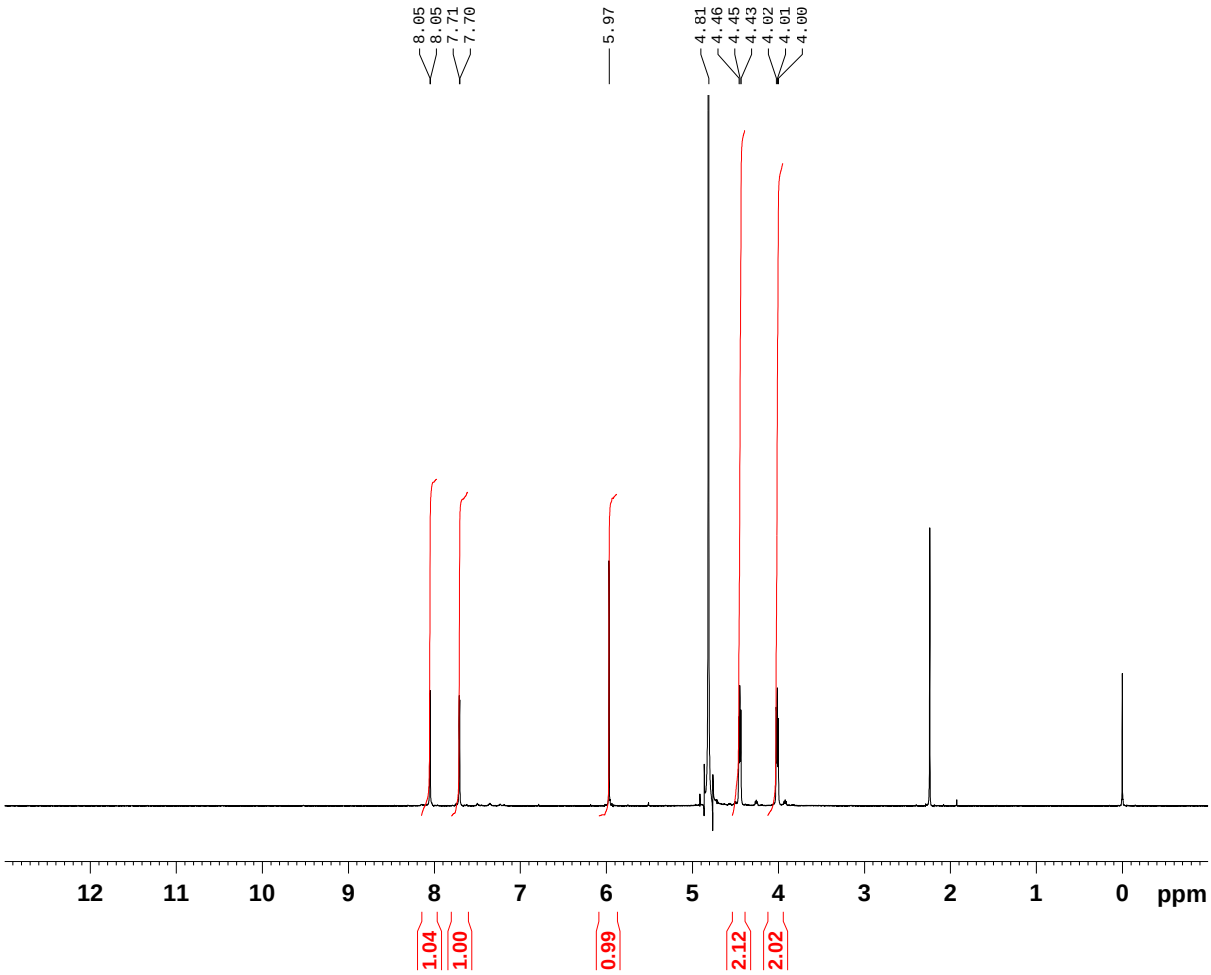


DEPT (100 MHz, D_2O)

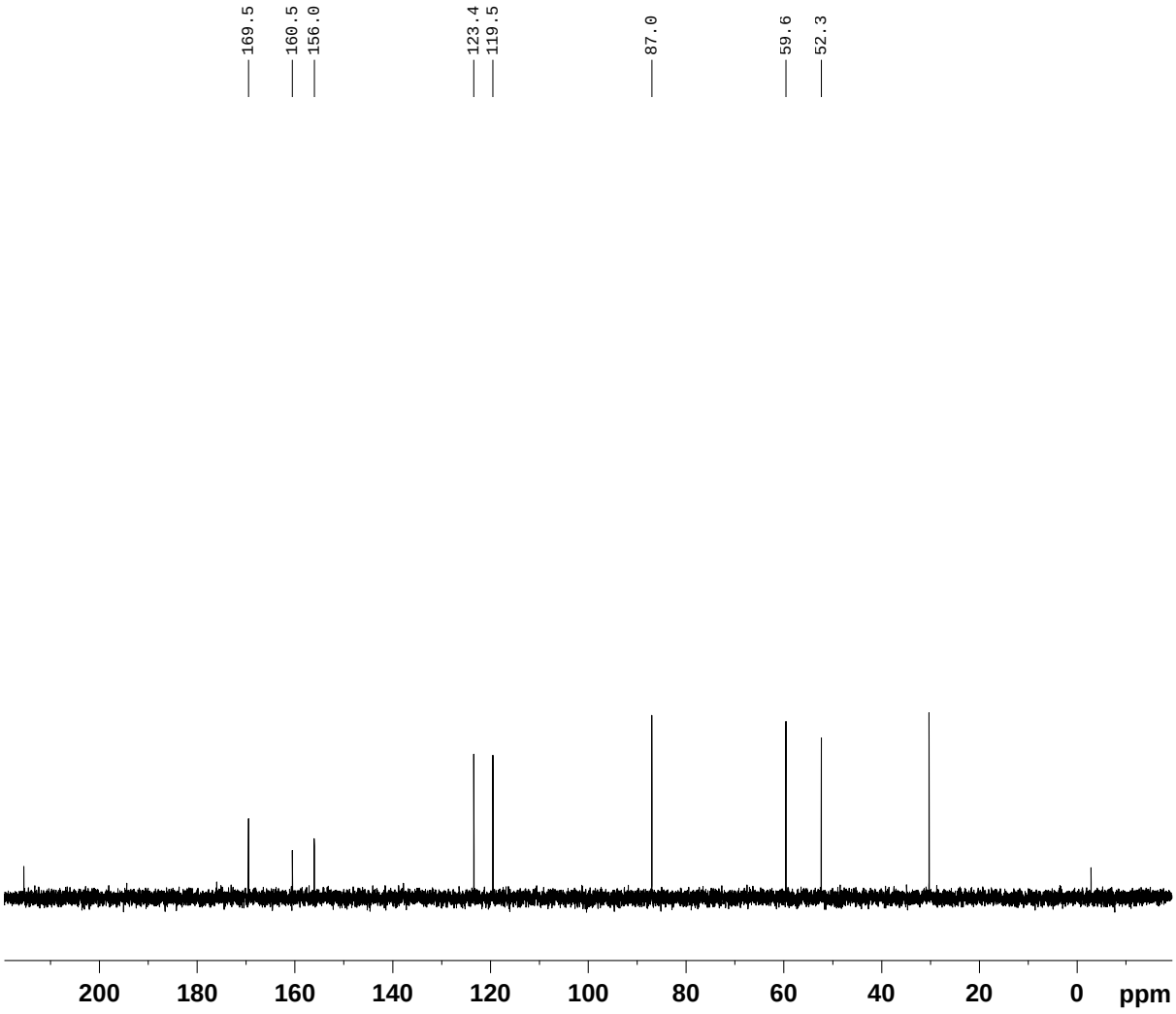


6-(3-(2-Hydroxyethyl)-imidazolio)-2,4(1*H*,3*H*)-pyrimidinedionate 2b

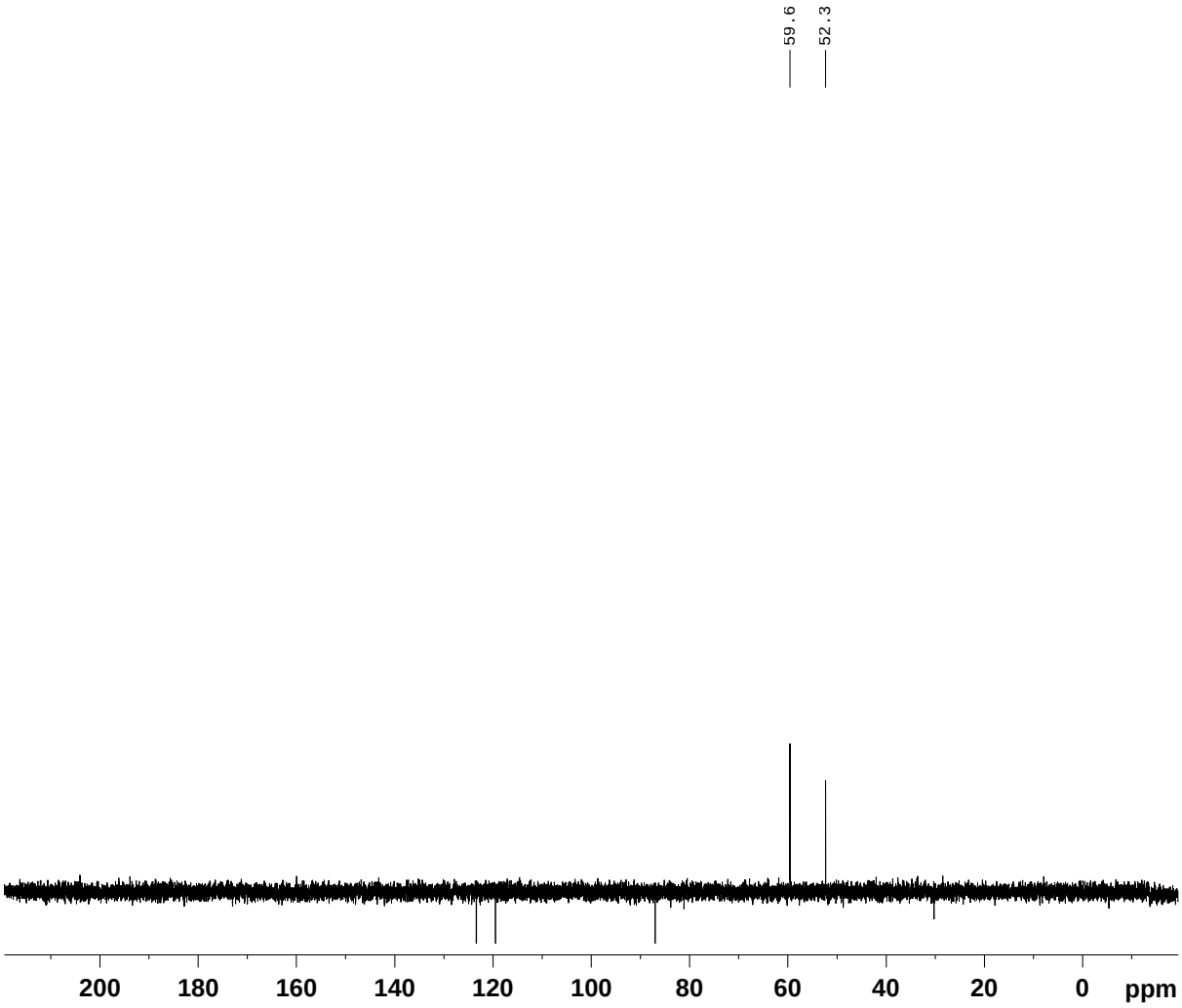
^{1}H NMR (400 MHz, D_2O)



^{13}C NMR (100 MHz, D_2O)

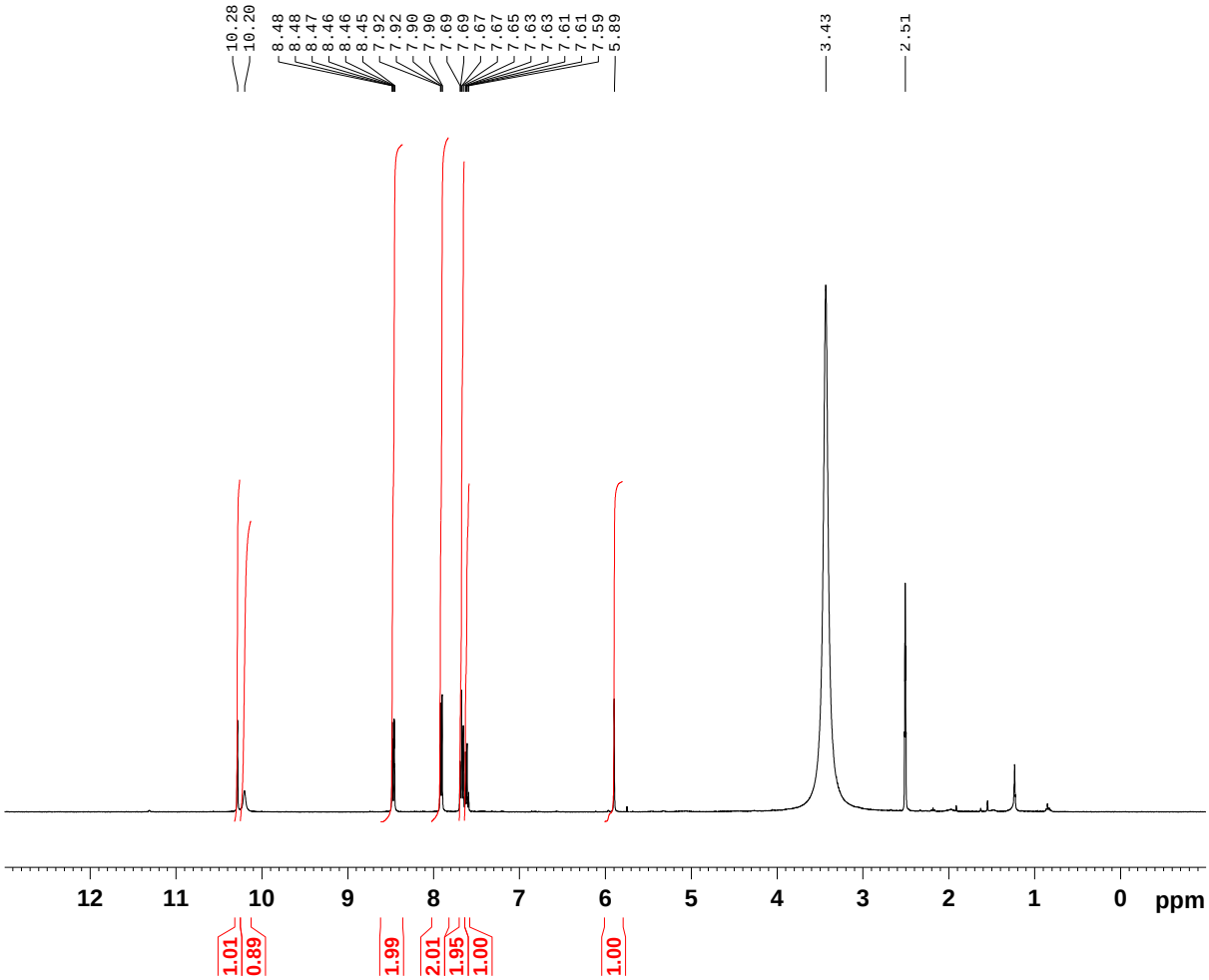


DEPT (100 MHz, D_2O)

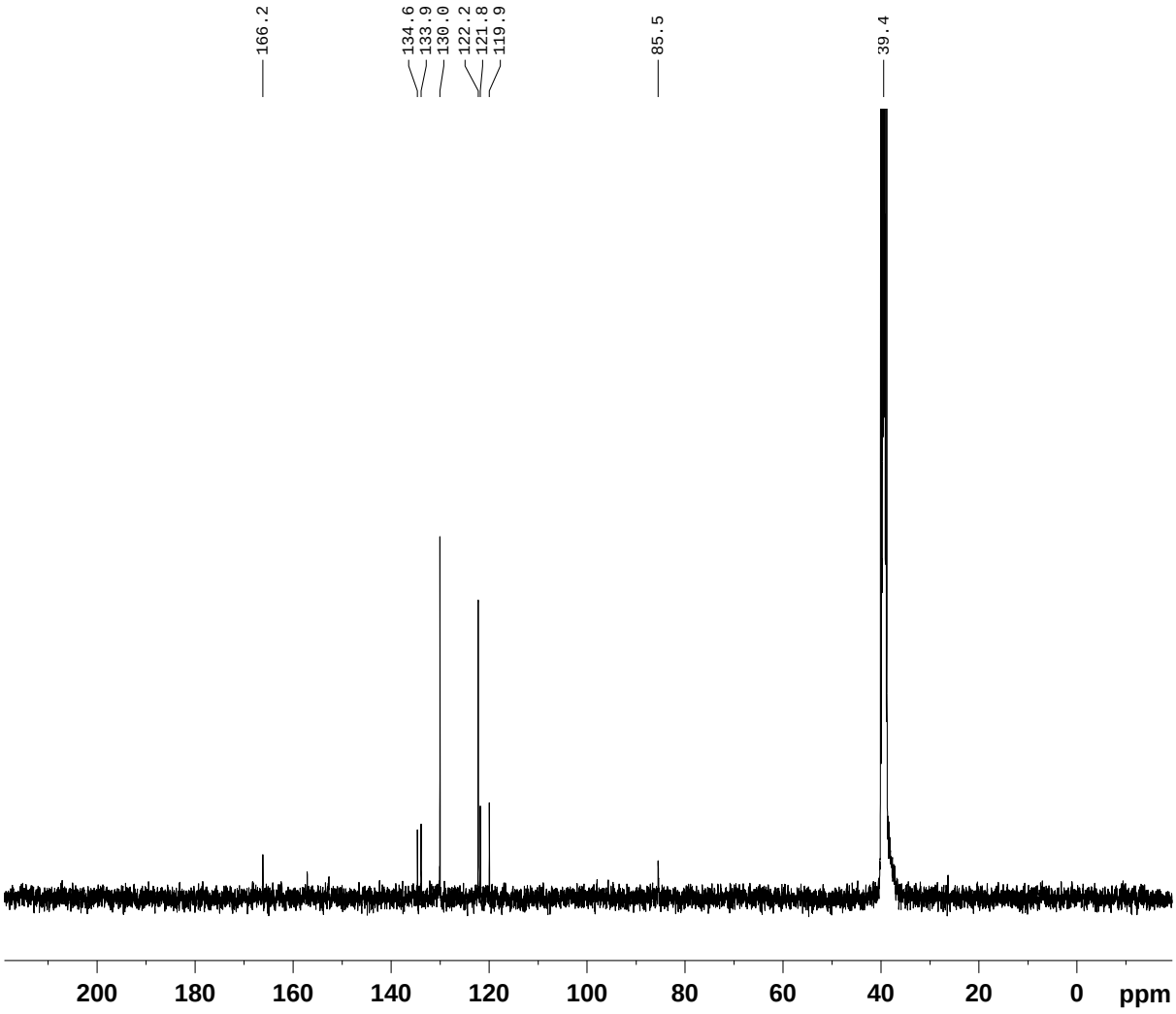


6-(3-Phenylimidazolio)-2,4(1*H*,3*H*)-pyrimidinedionate 2c

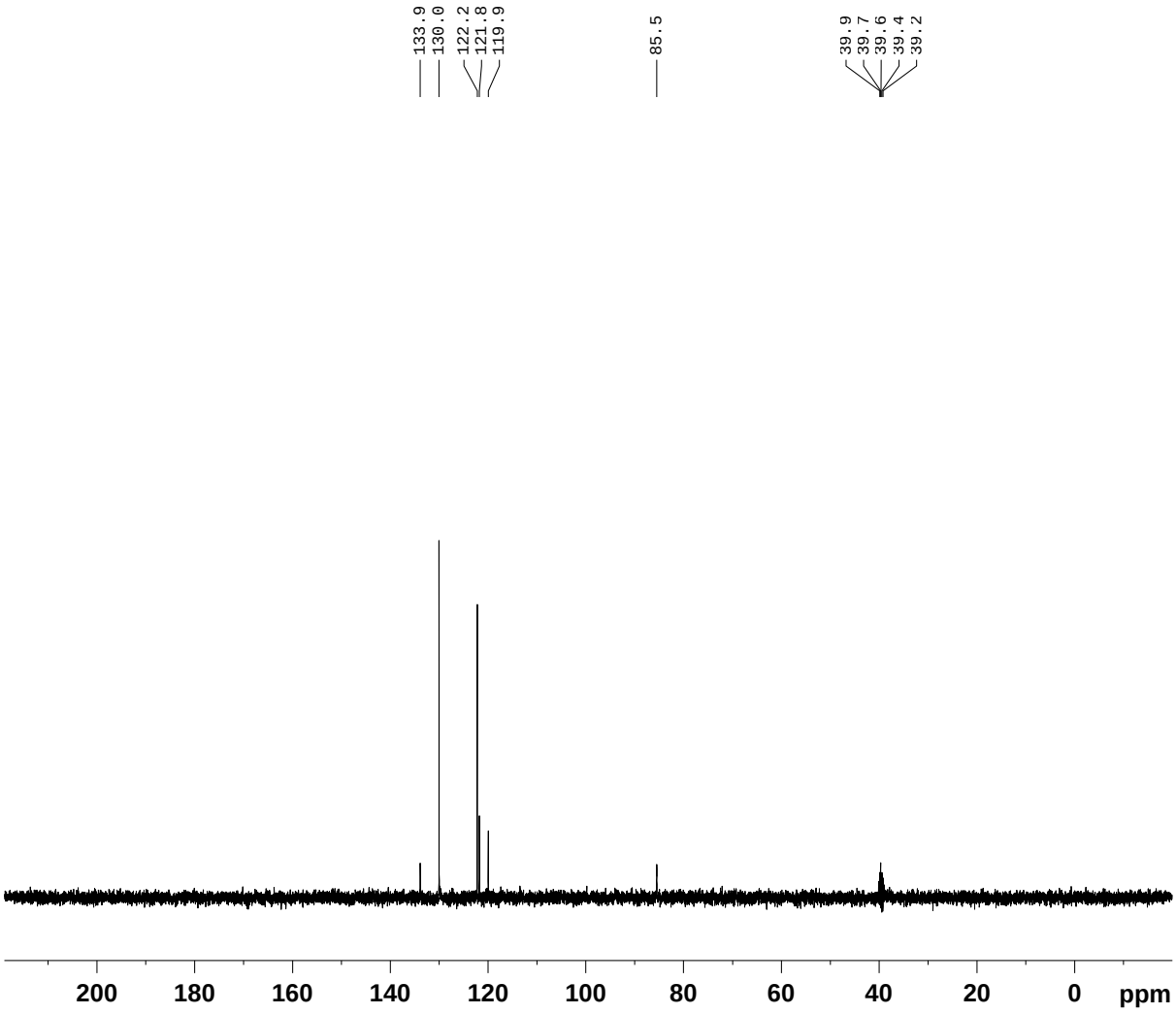
^{1}H NMR (400 MHz, DMSO-d$_6$)



^{13}C NMR (100 MHz, DMSO-d_6)

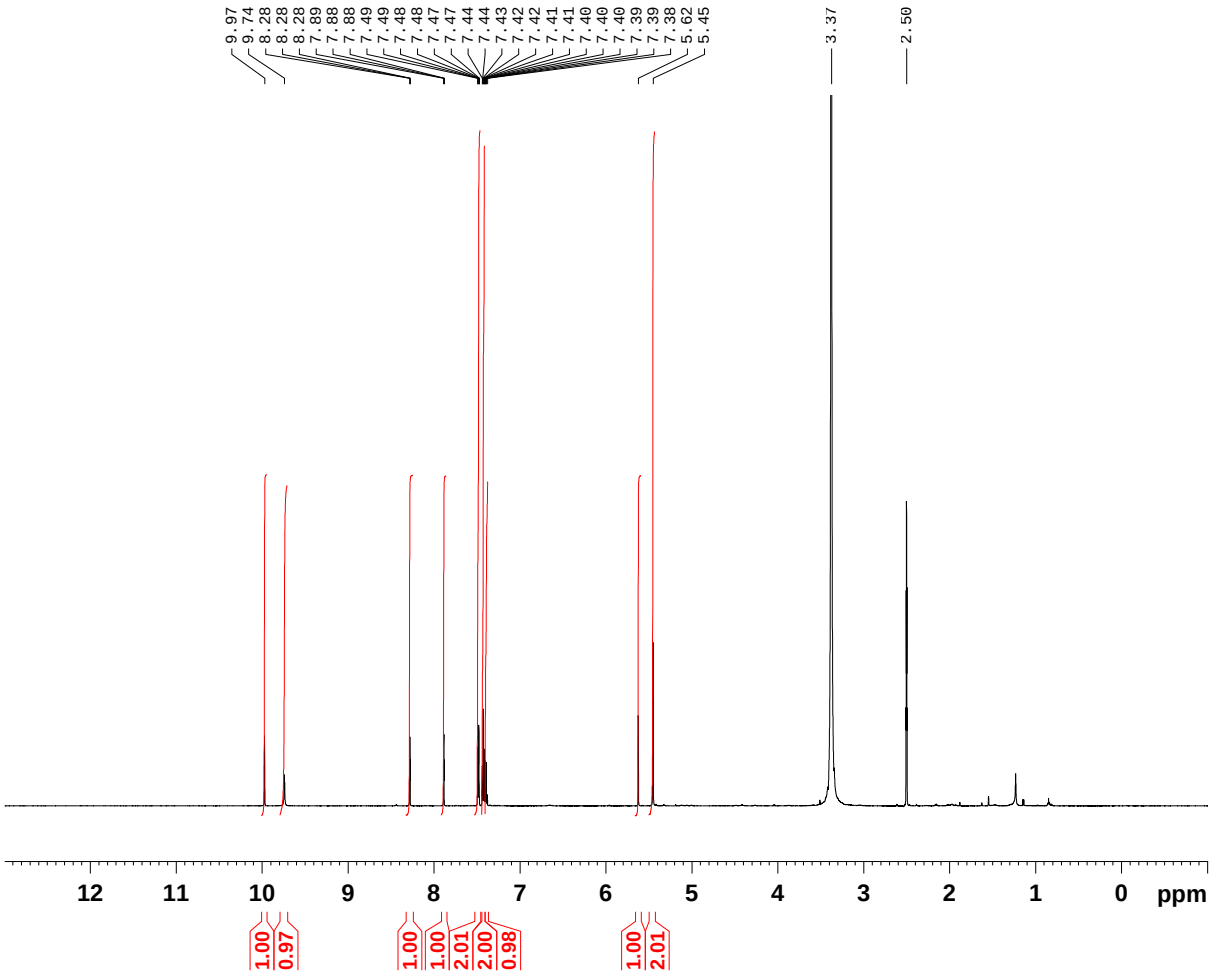


DEPT (100 MHz, DMSO-d_6)

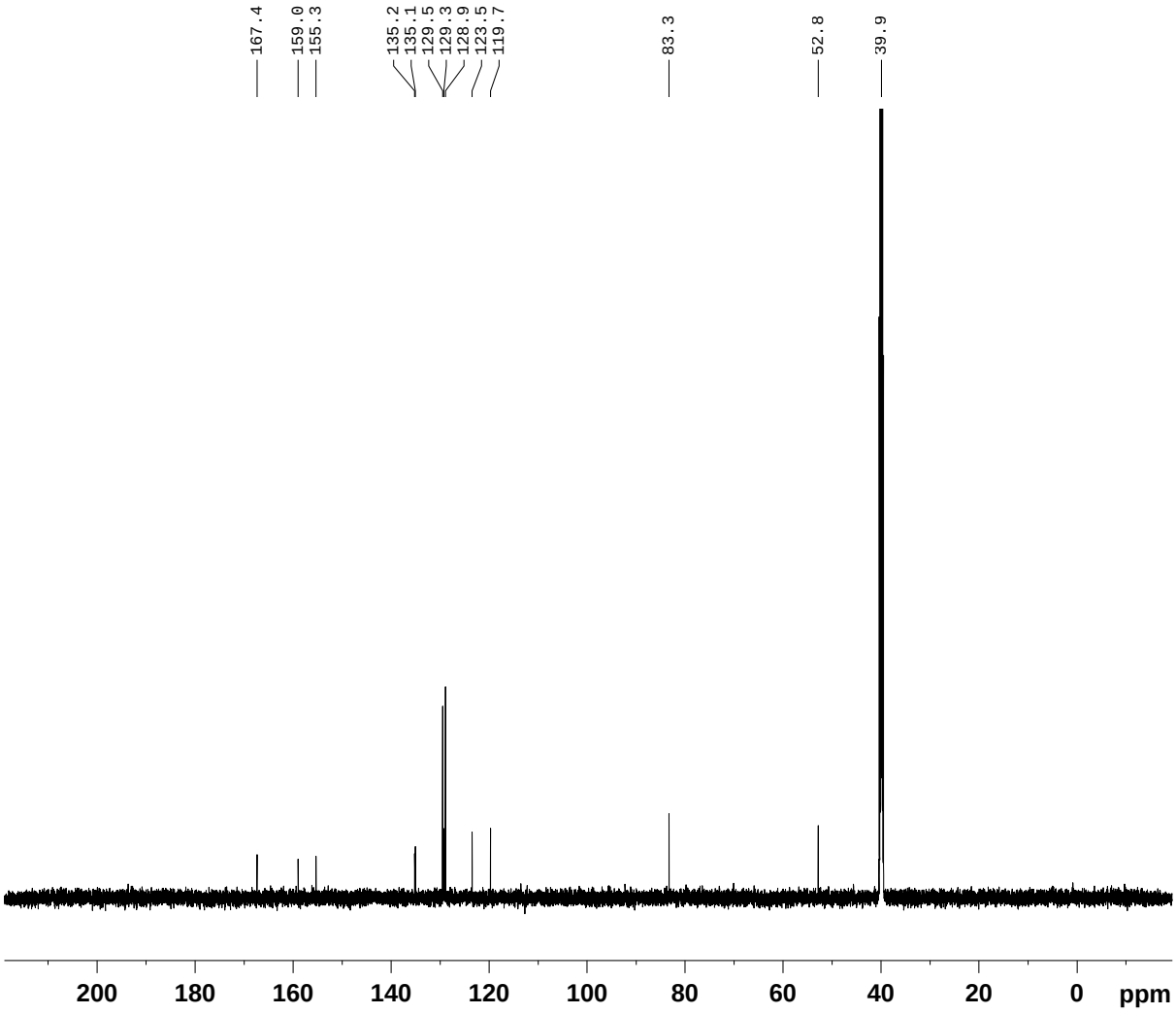


6-(3-Benzylimidazolio)-2,4(1*H*,3*H*)-pyrimidinedionate 2d

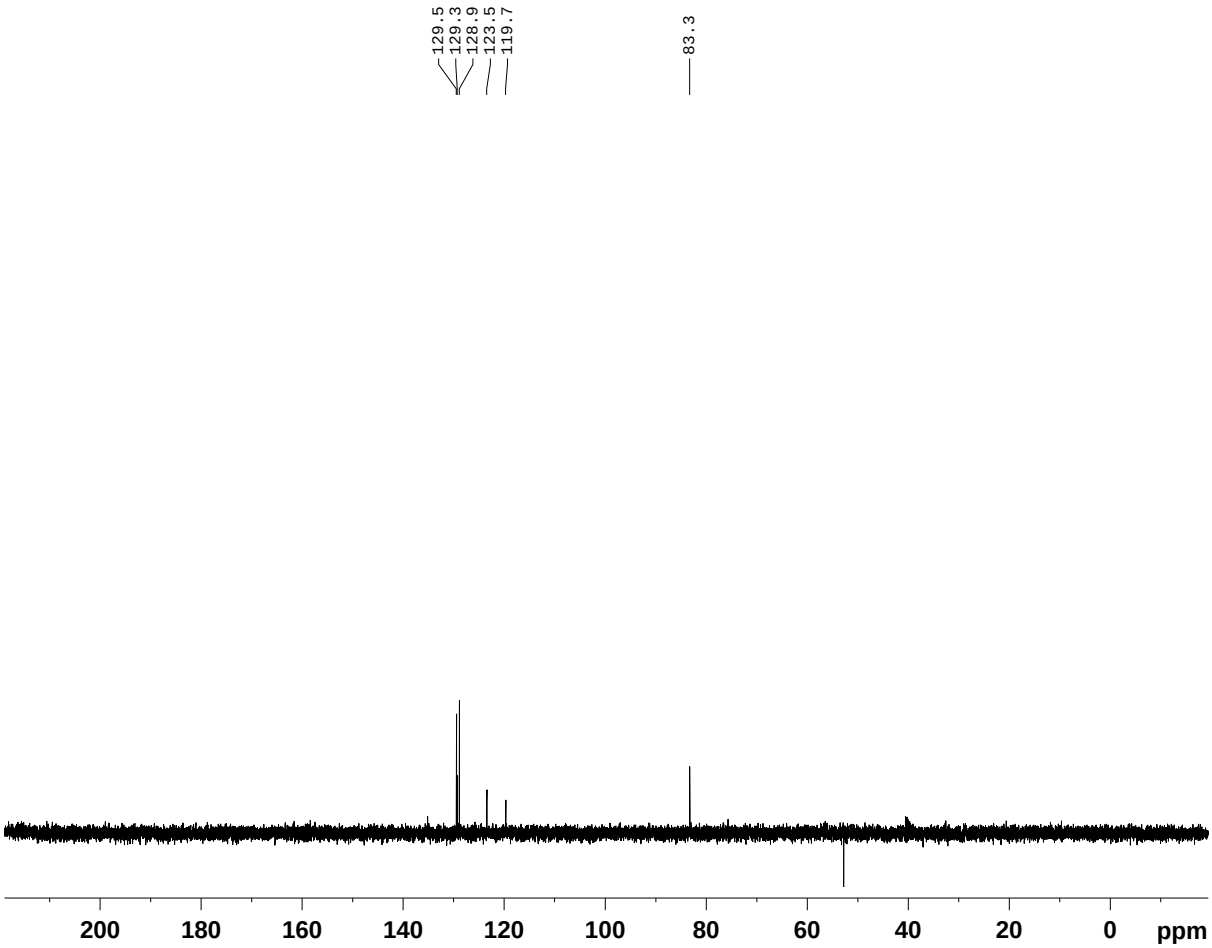
^{1}H NMR (400 MHz, DMSO-d$_6$)



^{13}C NMR (100 MHz, DMSO-d_6)

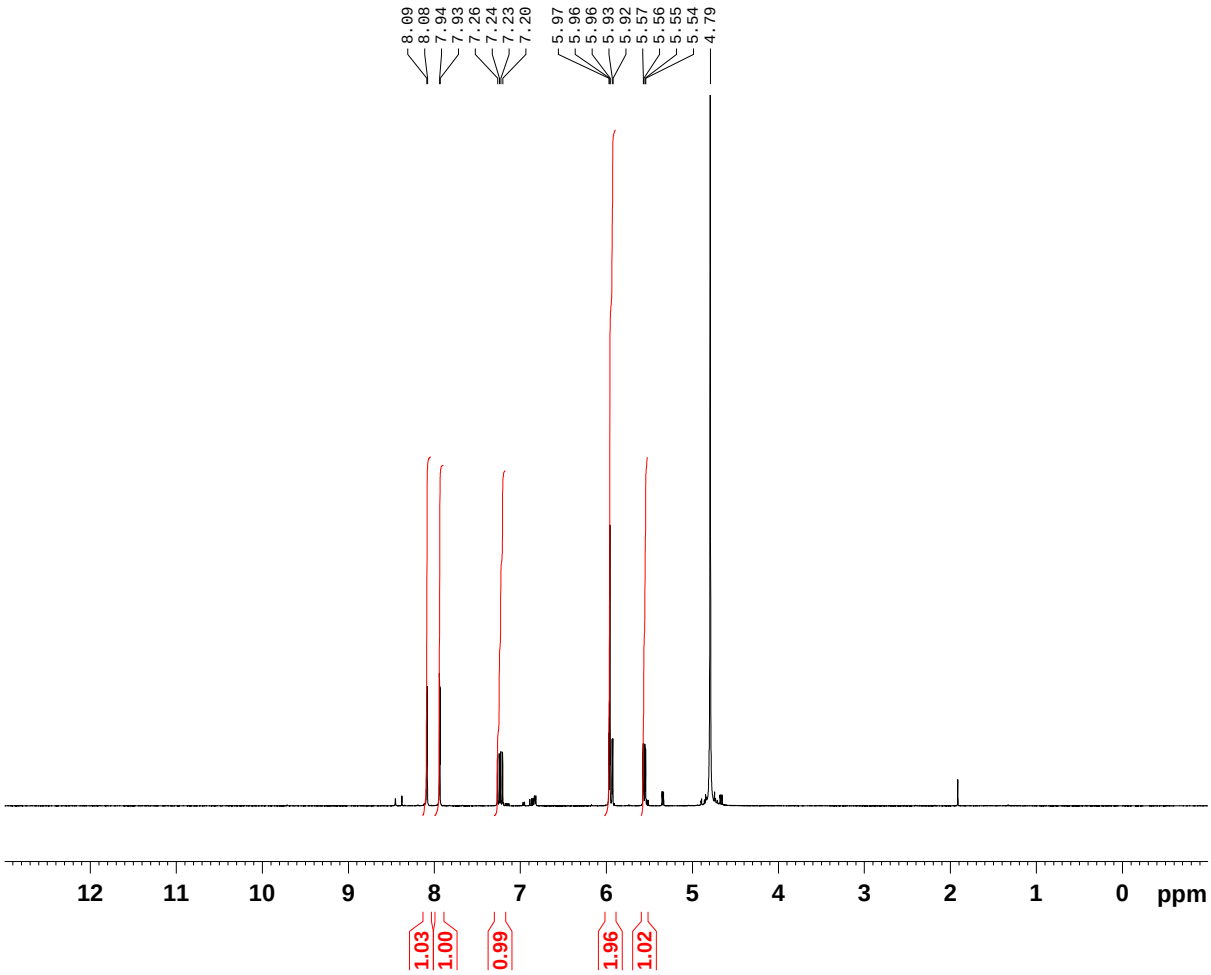


DEPT (100 MHz, DMSO-d_6)

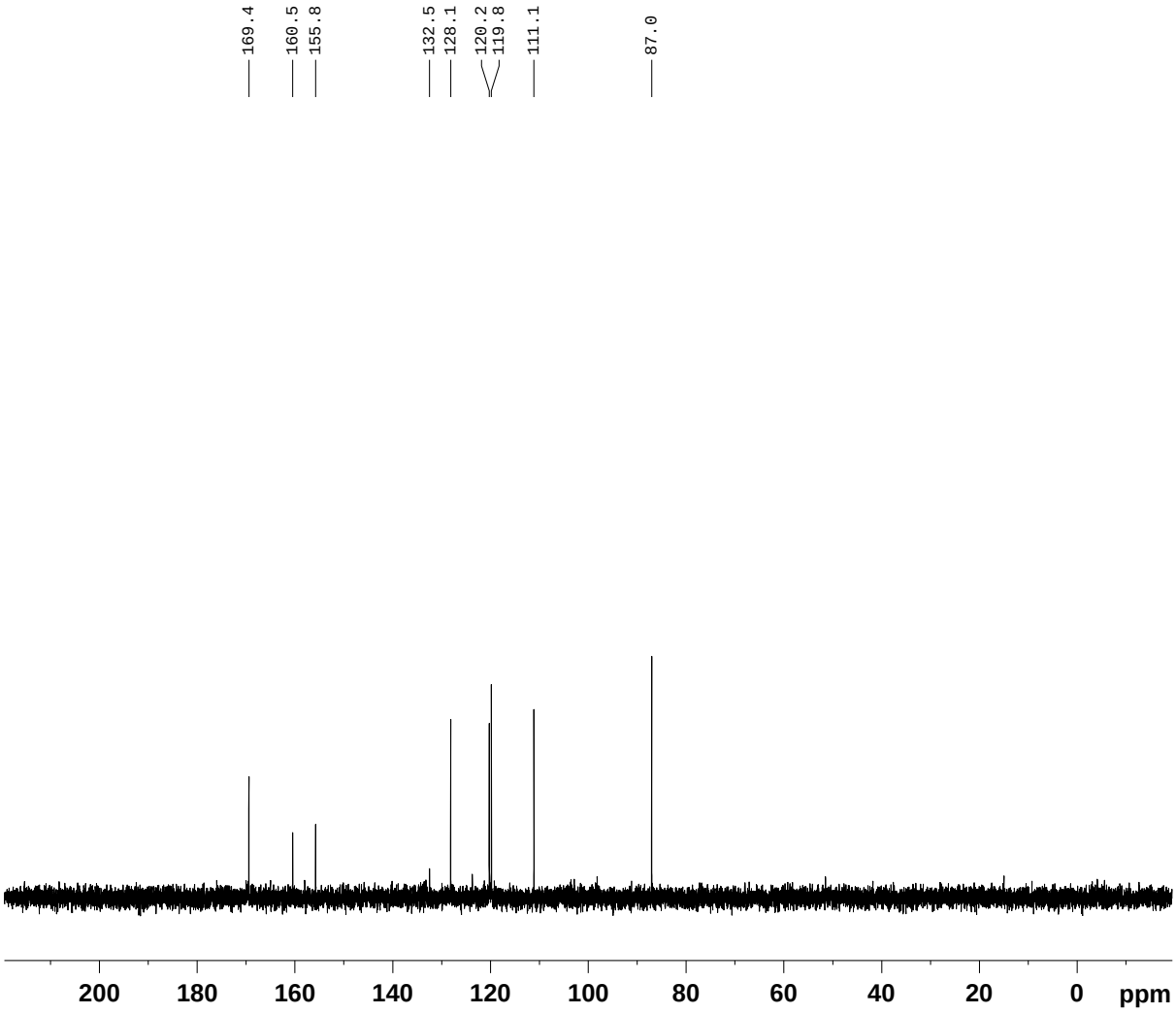


6-(3-Vinylimidazolio)-2,4(1*H*,3*H*)-pyrimidinedionate 2e

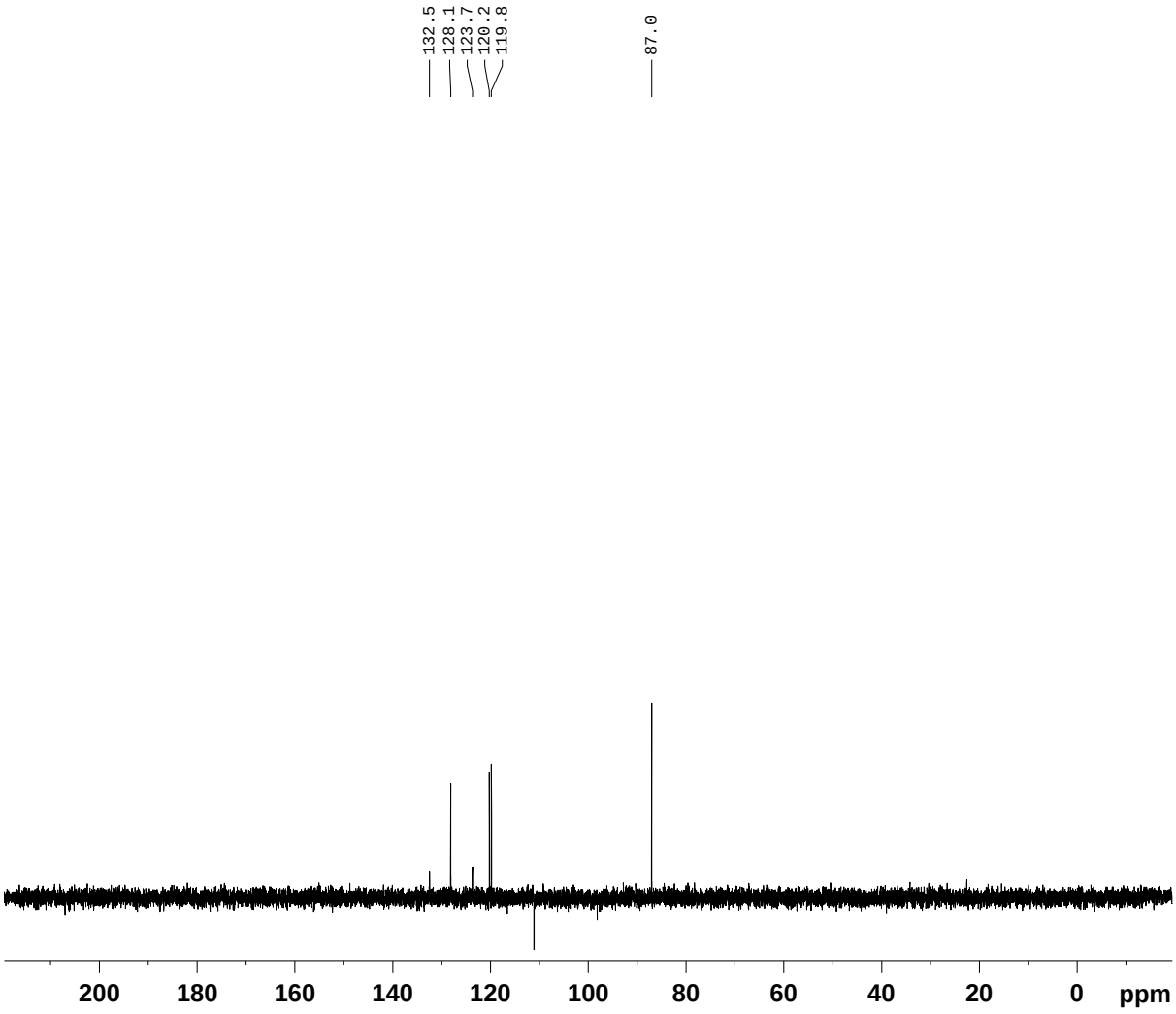
^{1}H NMR (400 MHz, D_2O)



^{13}C NMR (100 MHz, D_2O)

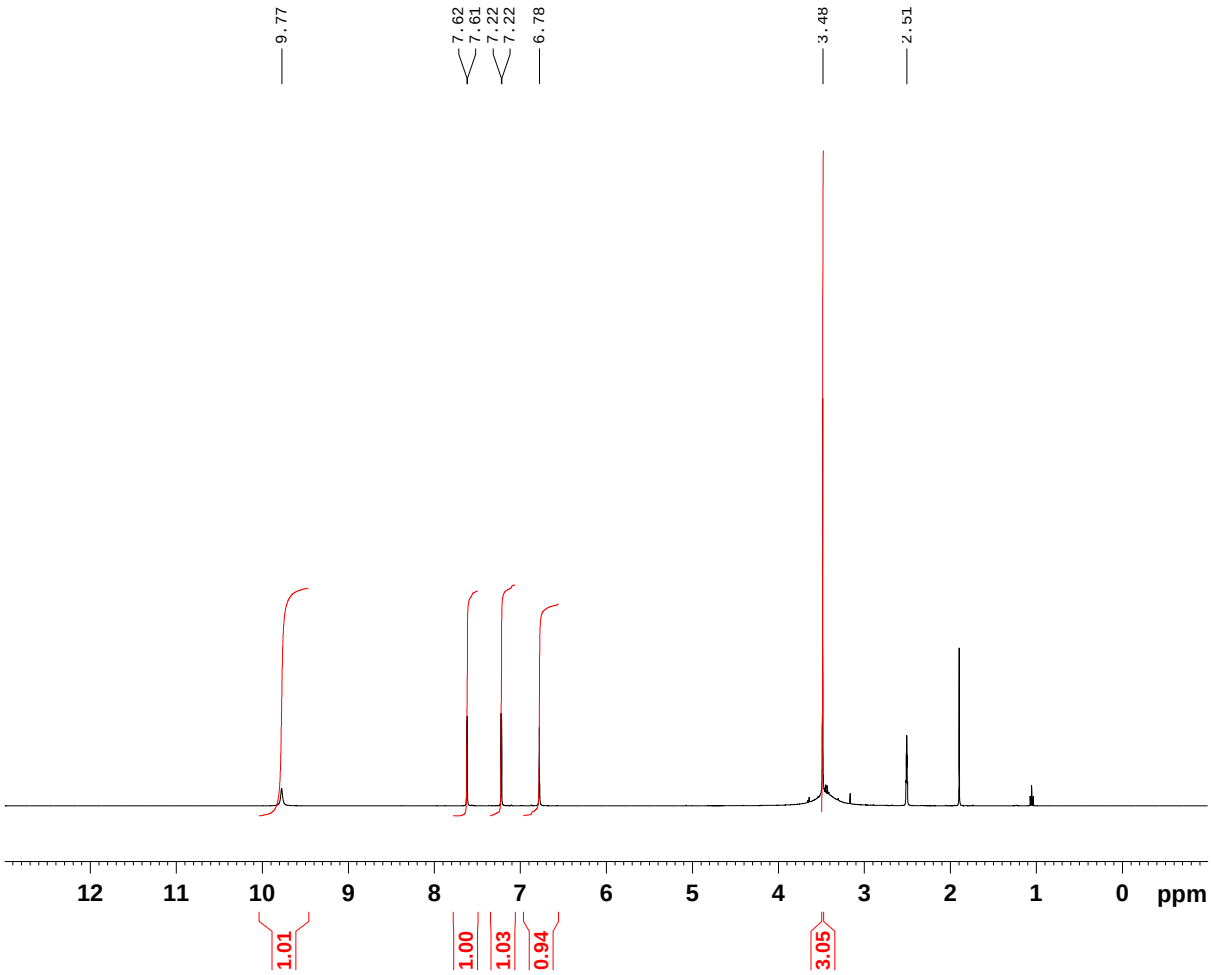


DEPT (100 MHz, D_2O)

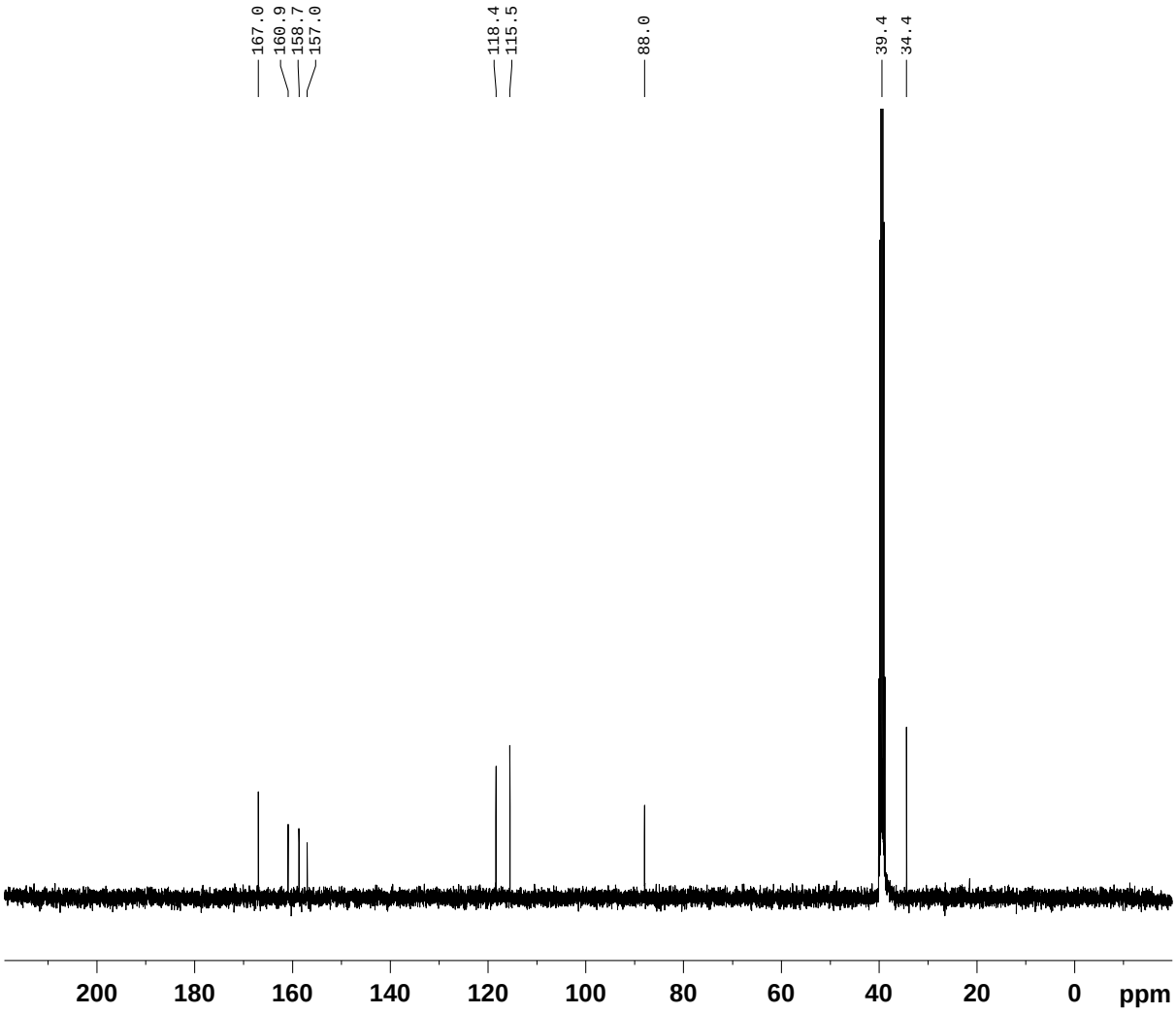


6-(3-Methyl-2-thioxo-2,3-dihydro-1*H*-imidazol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione 23

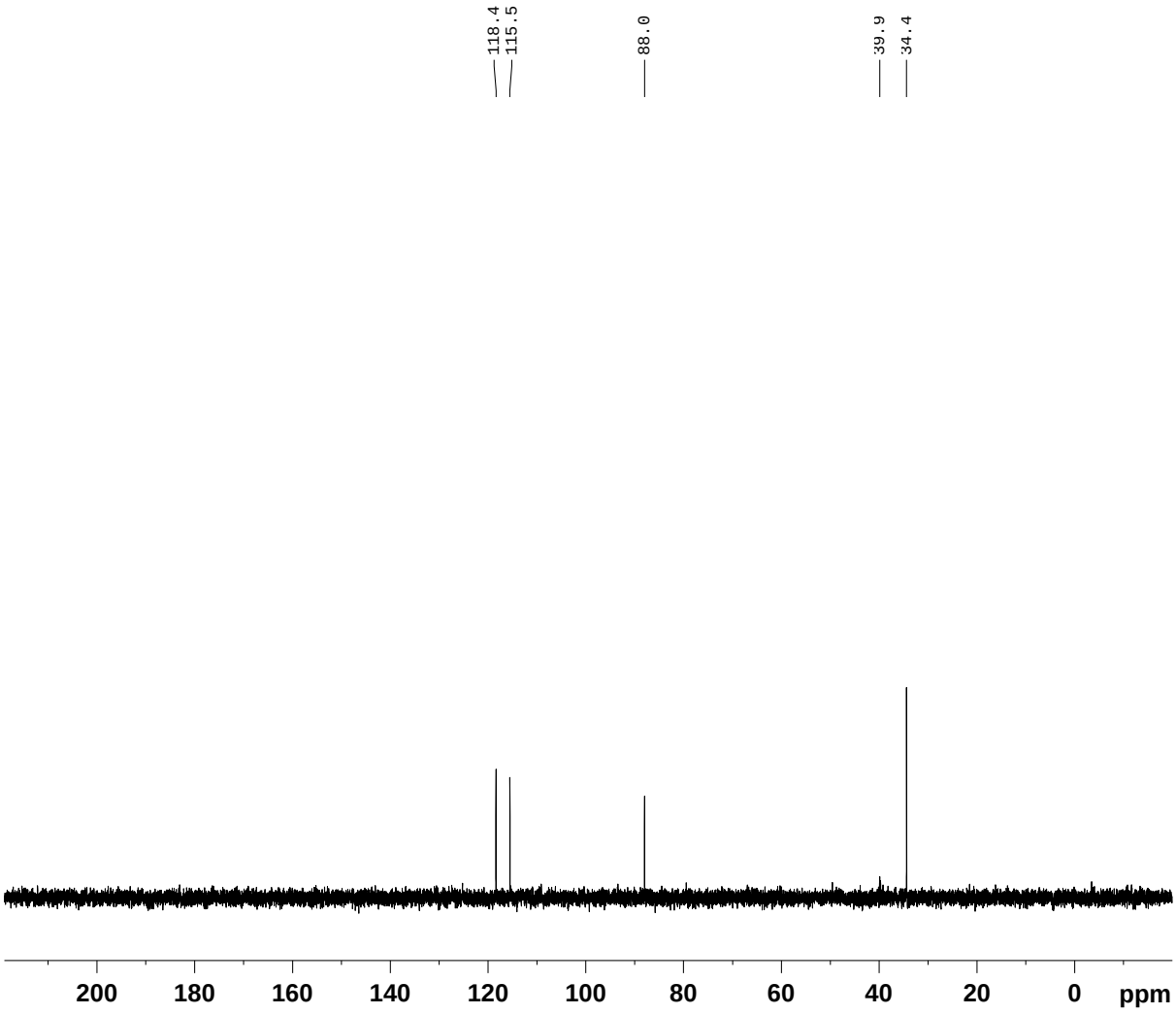
^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C NMR (100 MHz, DMSO-d_6)

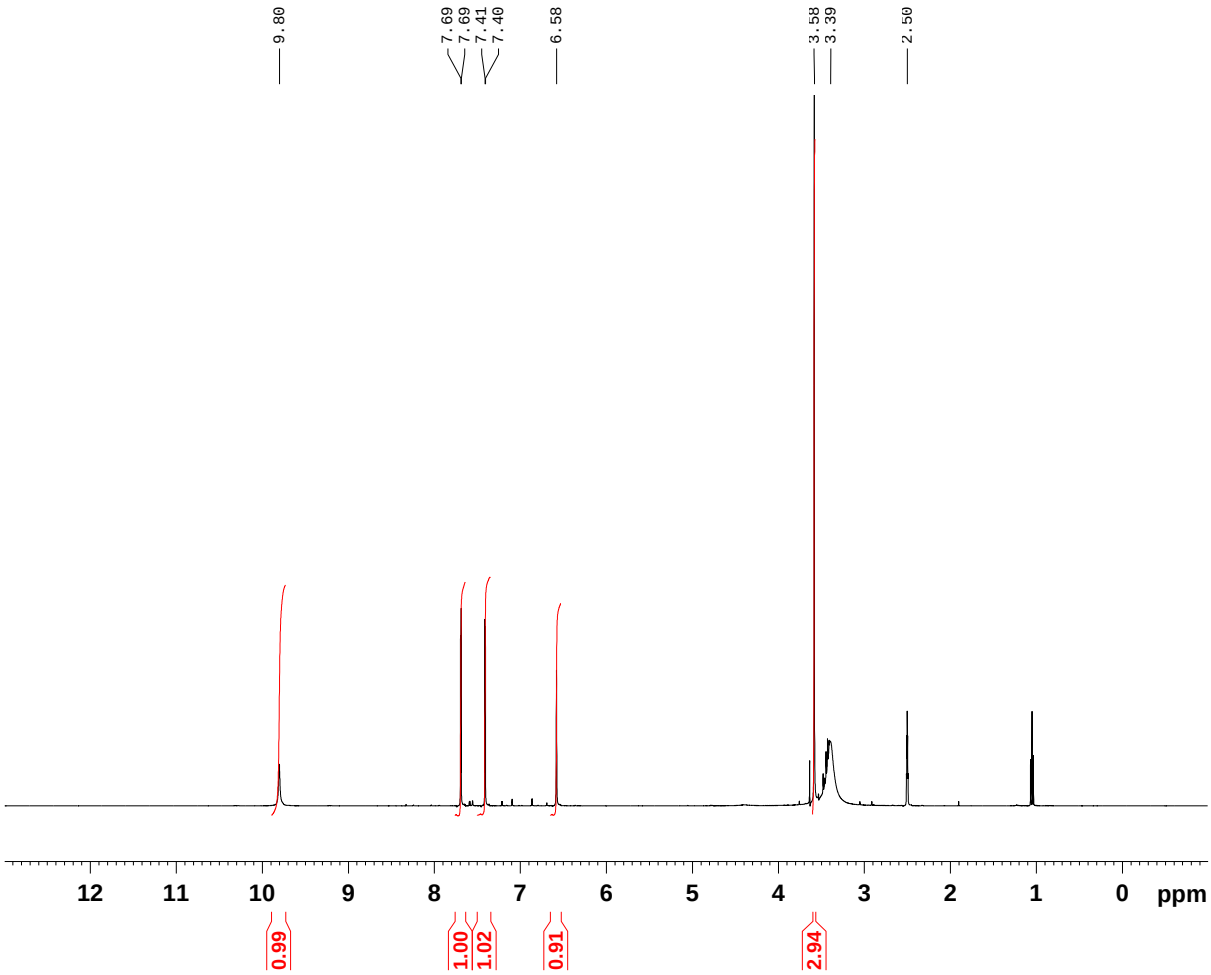


DEPT (100 MHz, DMSO-d_6)

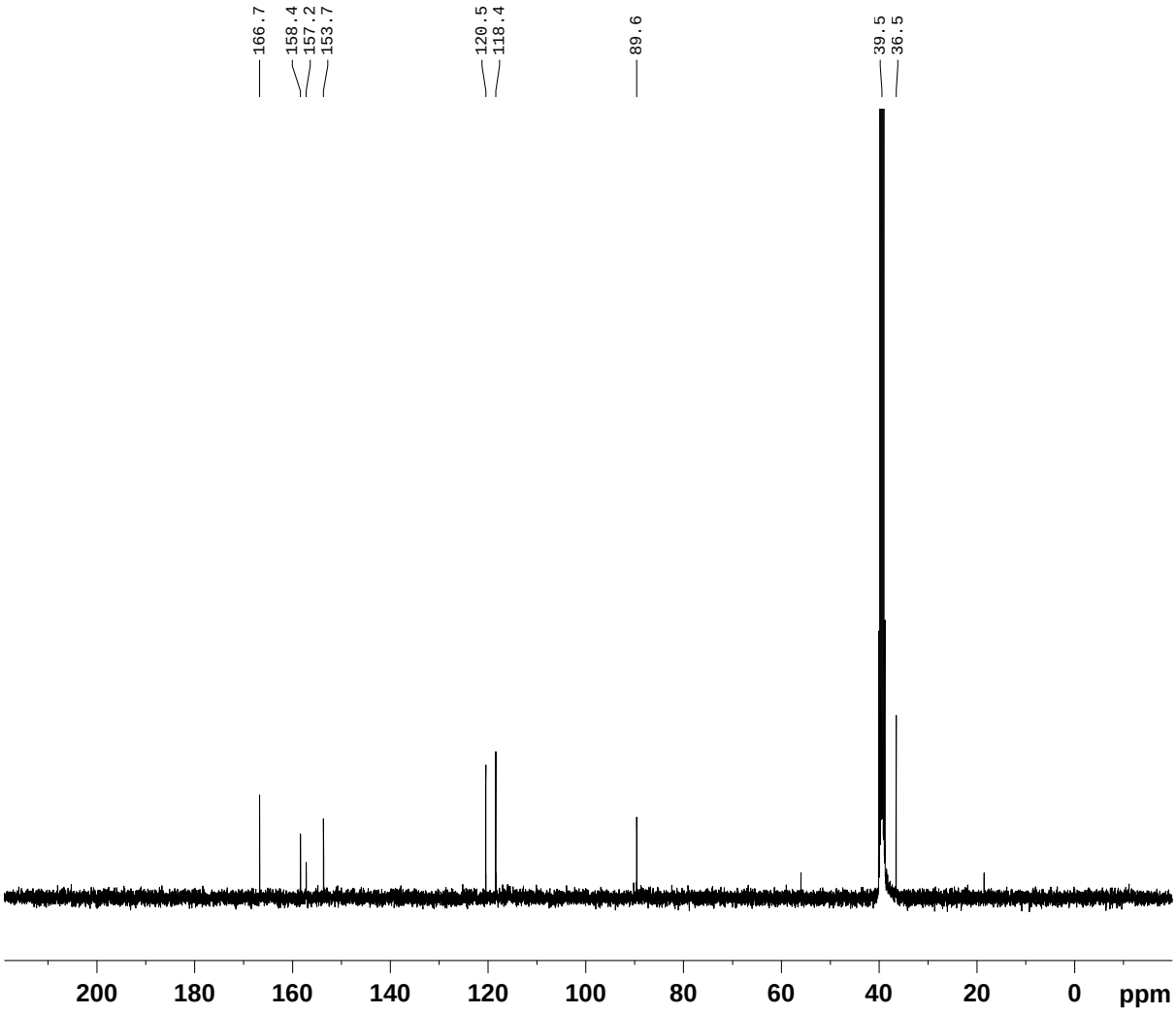


6-(3-Methyl-2-selenoxo-2,3-dihydro-1*H*-imidazol-1-yl)pyrimidine-2,4(1*H*,3*H*)-dione 24

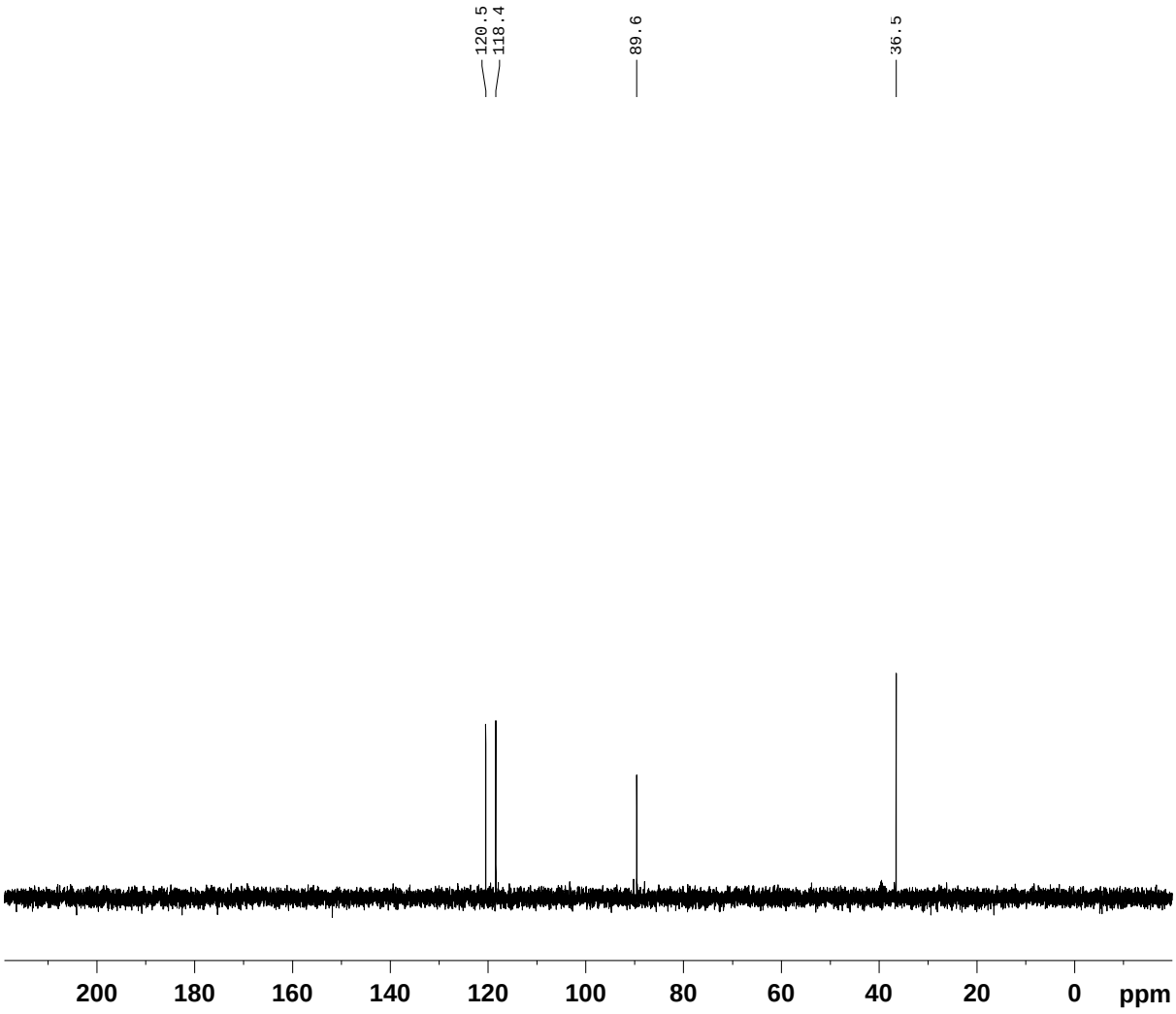
^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C NMR (100 MHz, DMSO-d_6)

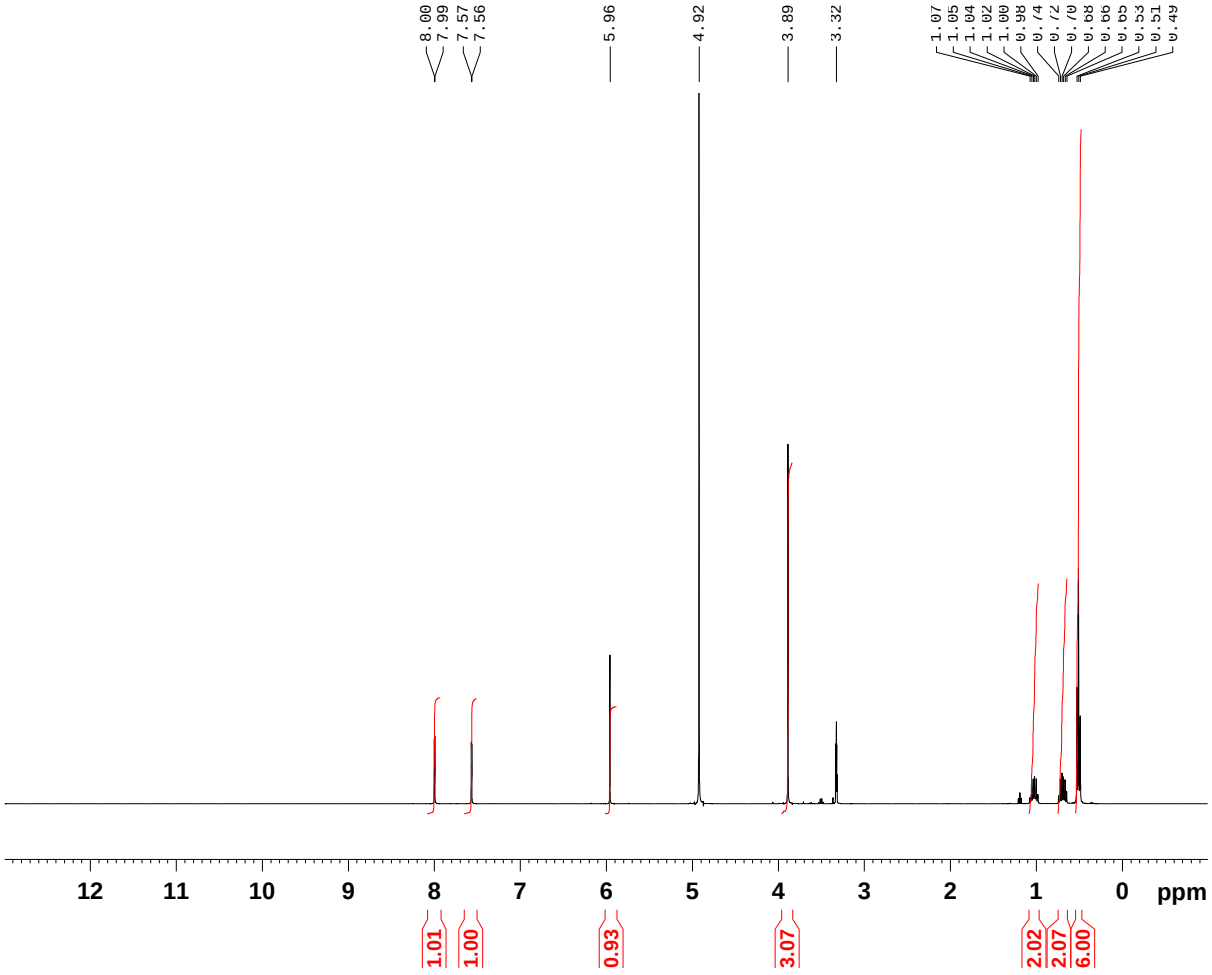


DEPT (100 MHz, DMSO-d_6)

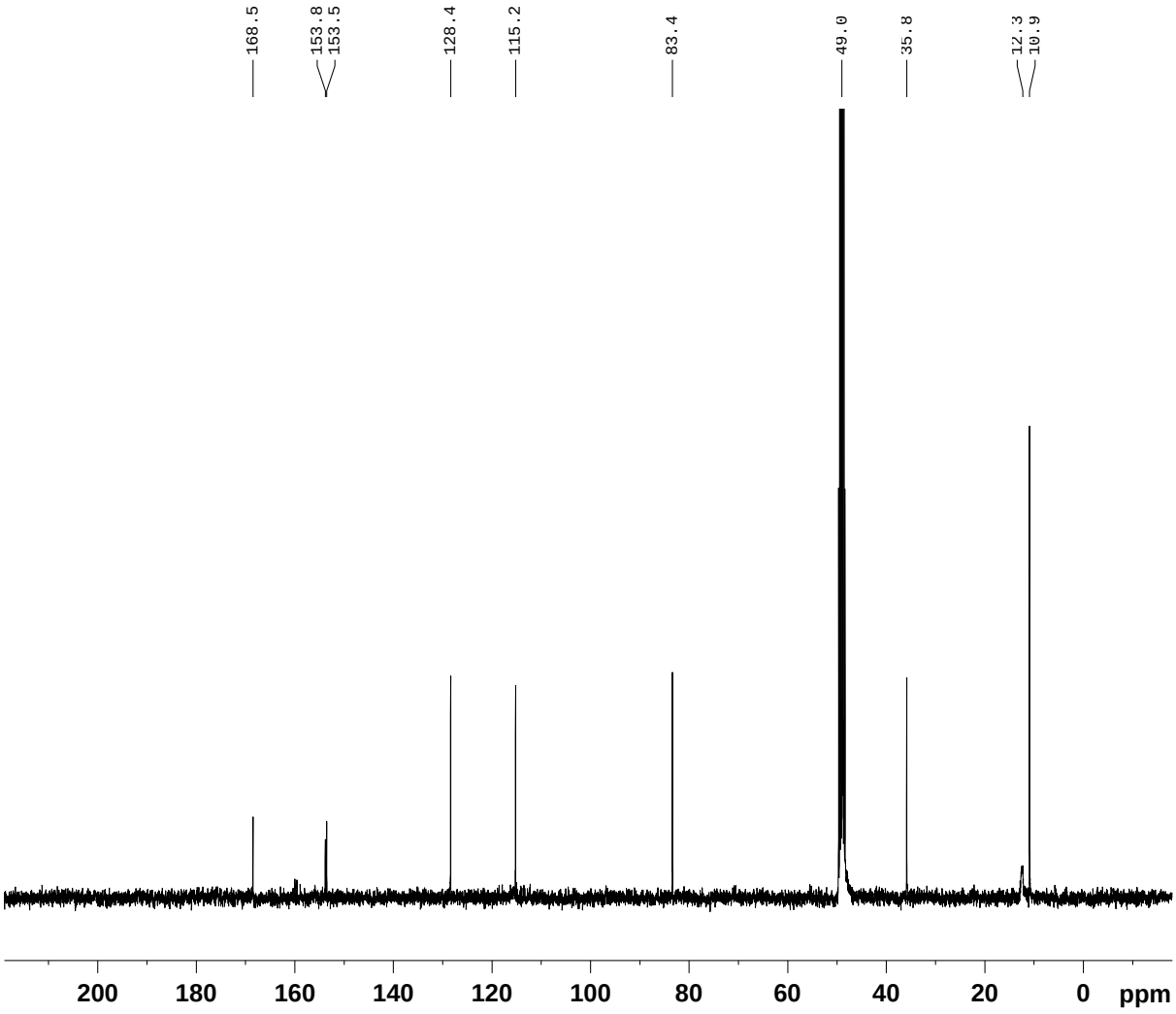


10,10-Diethyl-1-methyl-6,8-dioxo-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 25a

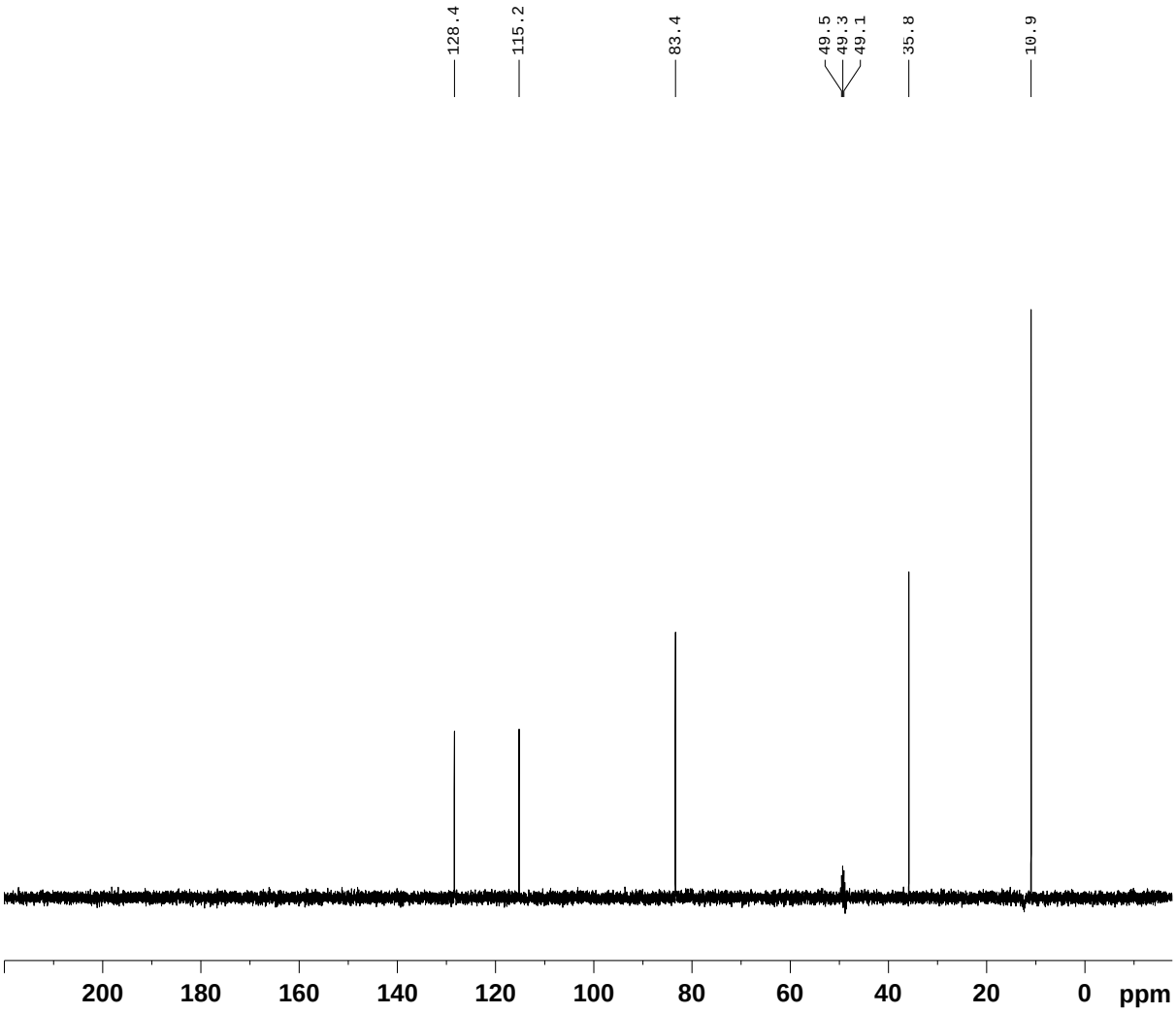
^{1}H NMR (400 MHz, CD_3OD)



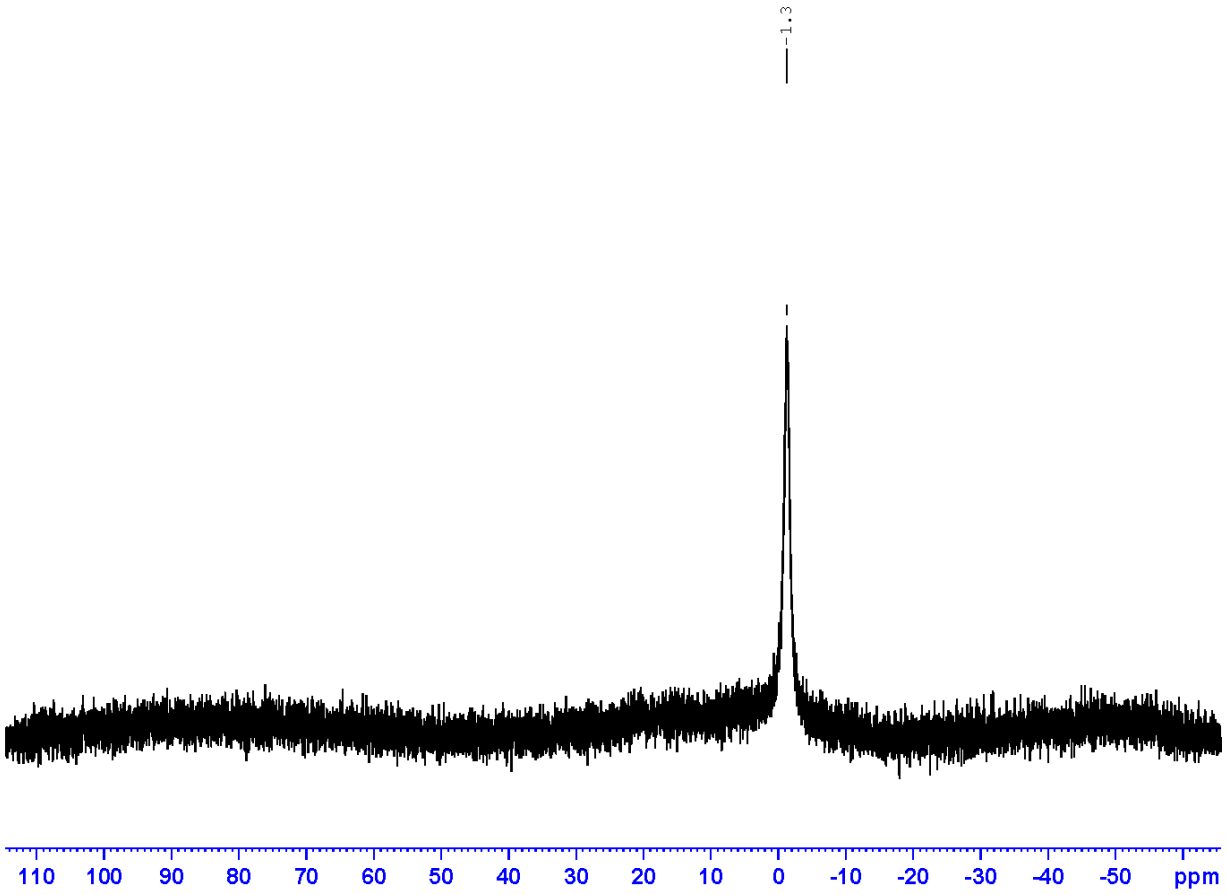
^{13}C NMR (100 MHz, CD_3OD)



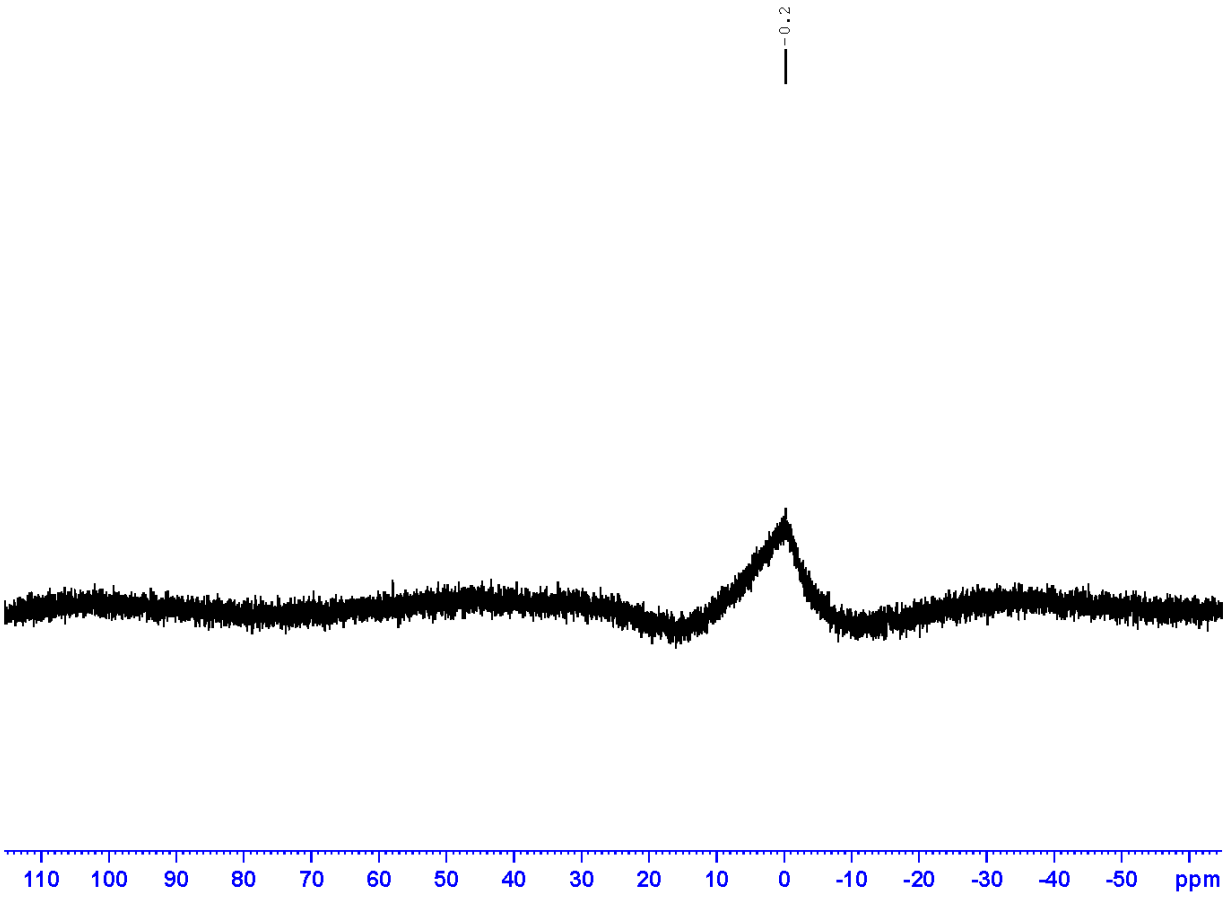
DEPT (100 MHz, CD_3OD)



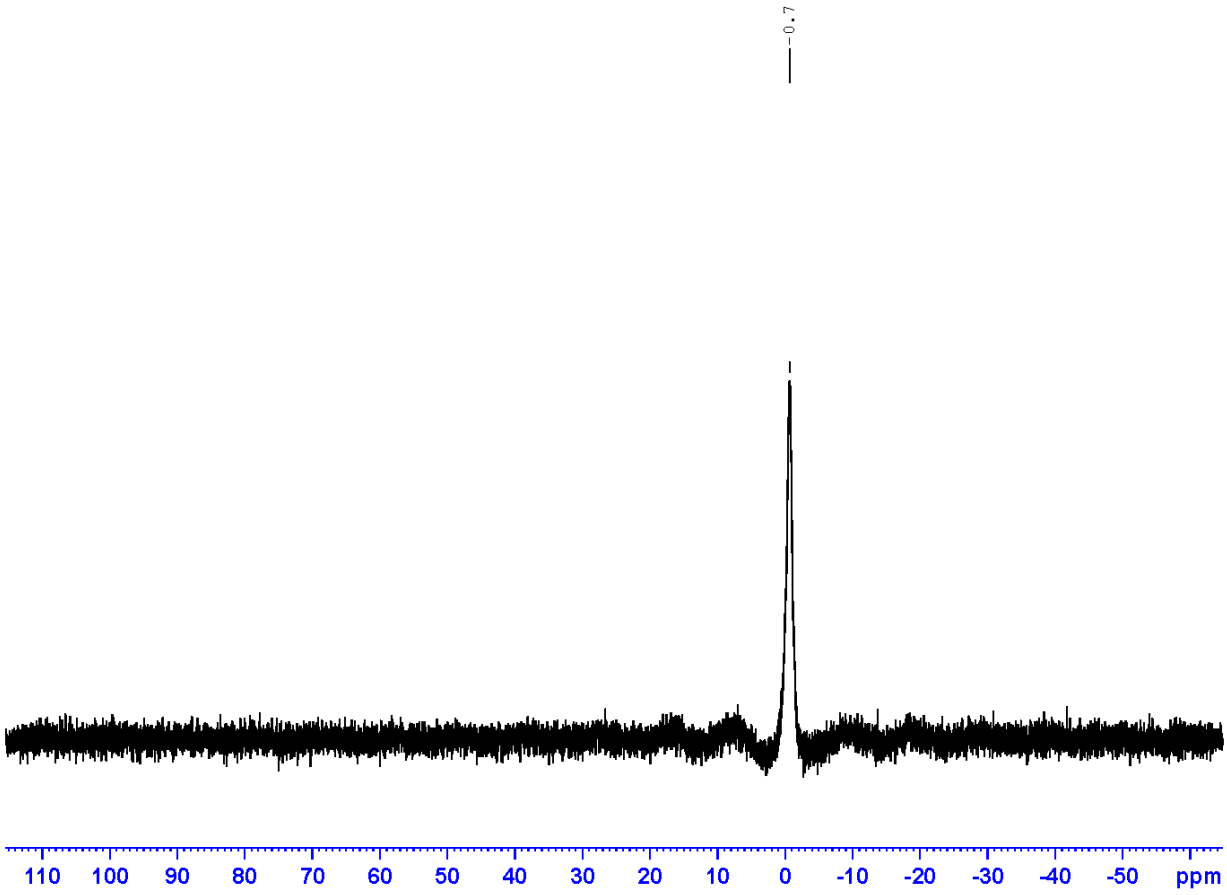
^{11}B NMR (192 MHz, CD_3CN)



^{11}B NMR (192 MHz, DMSO-d_6)

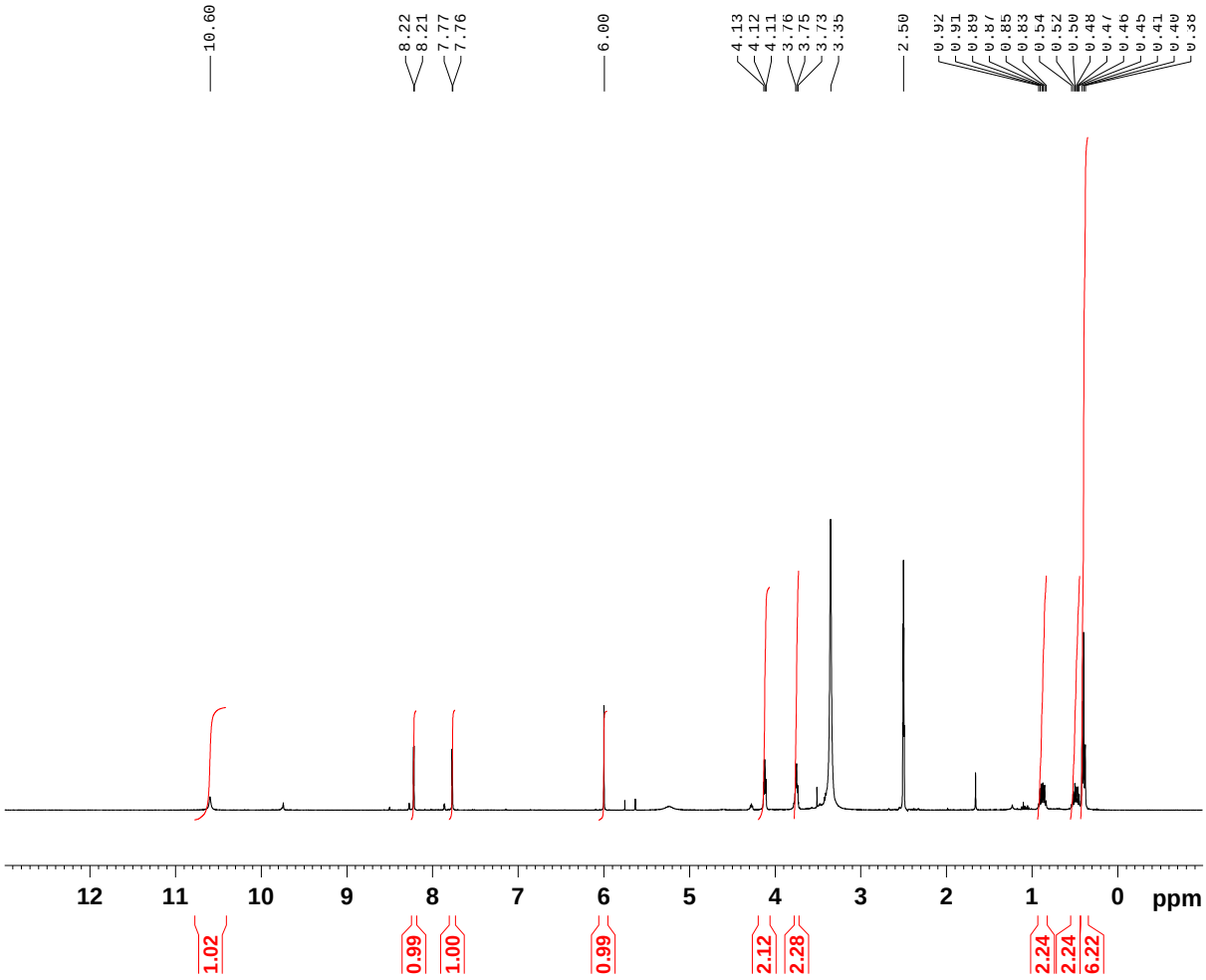


^{11}B NMR (192 MHz, THF-d_8)

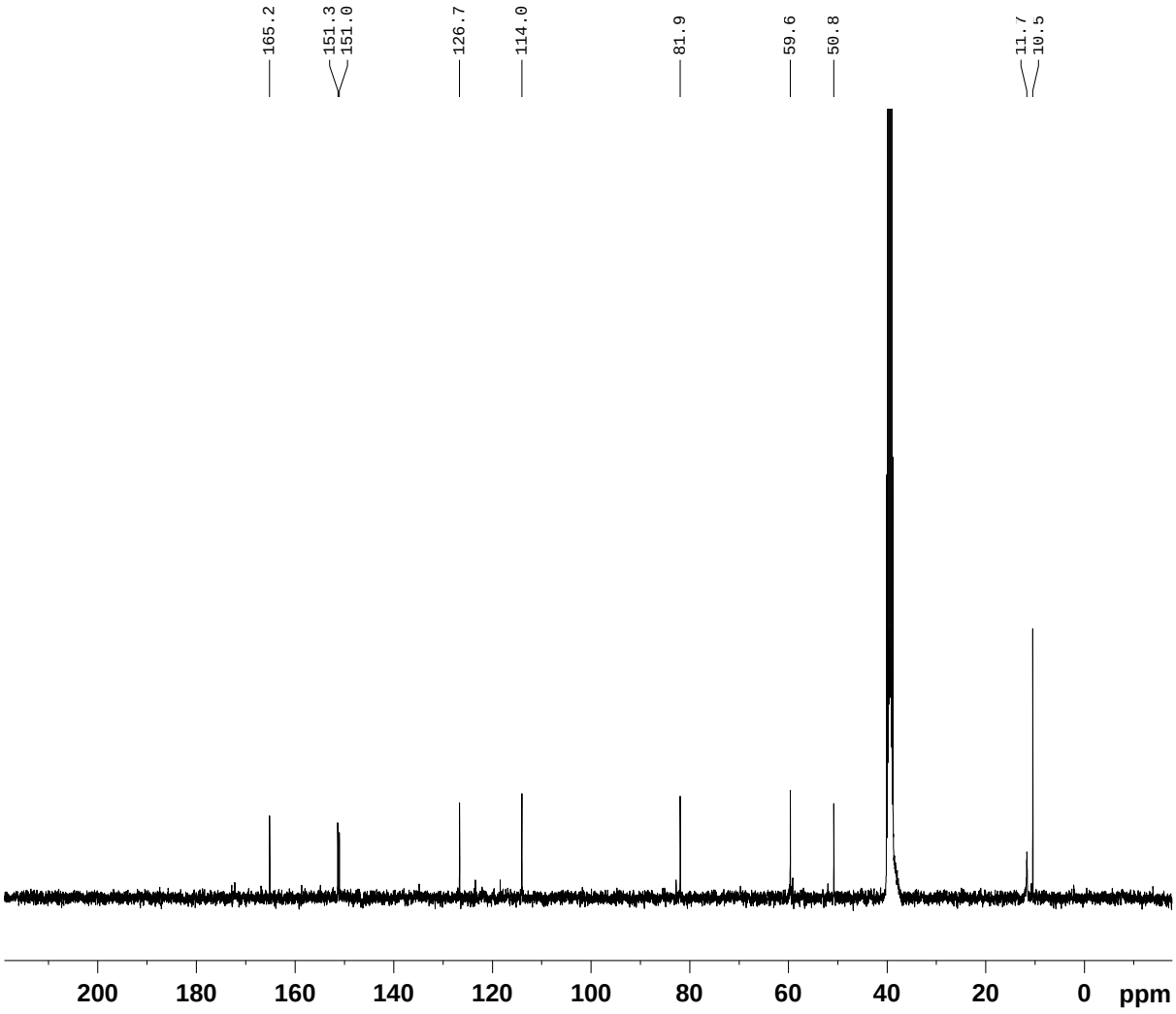


10,10-Diethyl-1-(hydroxymethyl)-6,8-dioxo-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 25b

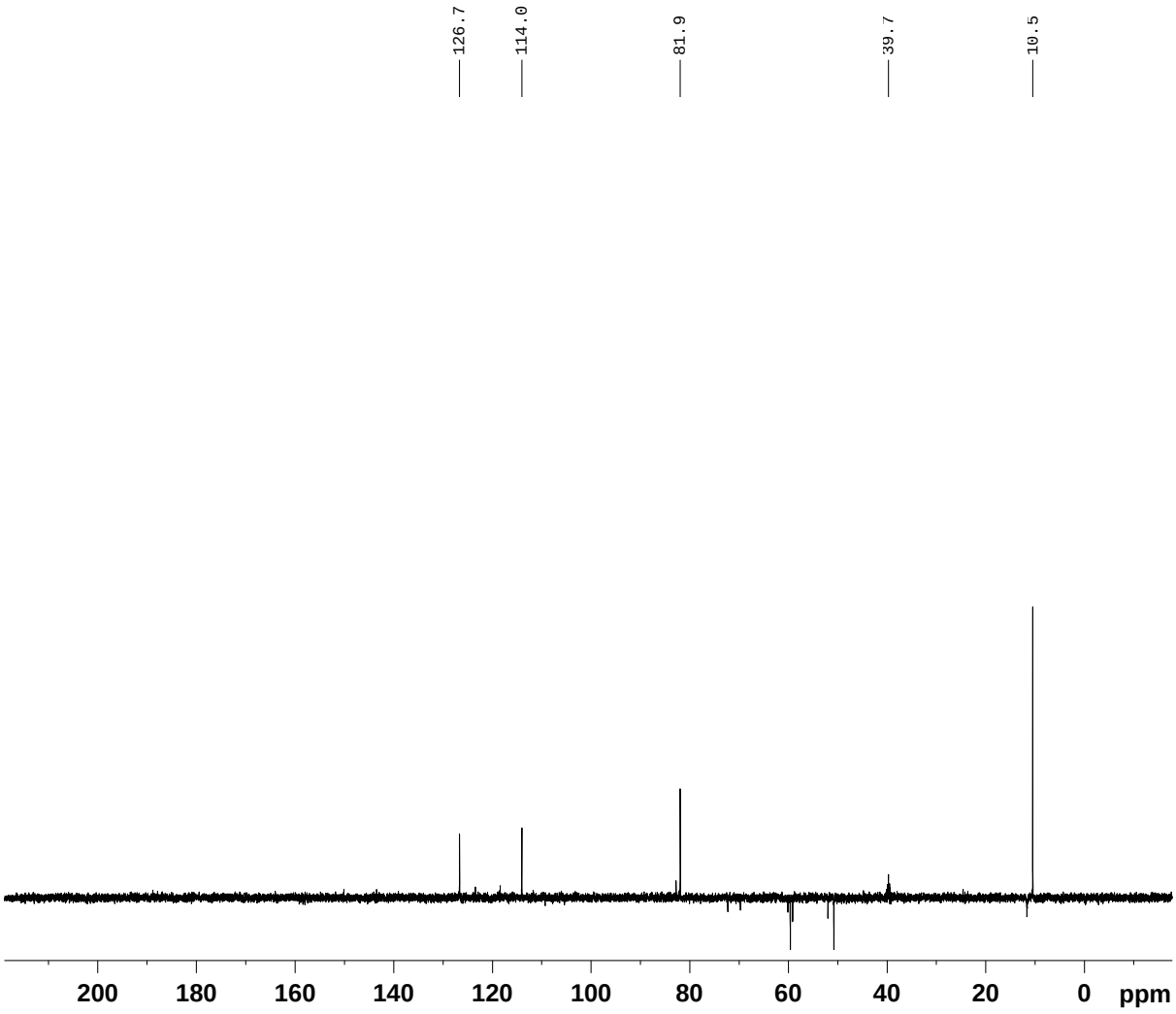
^{1}H NMR (400 MHz, DMSO-d_6)



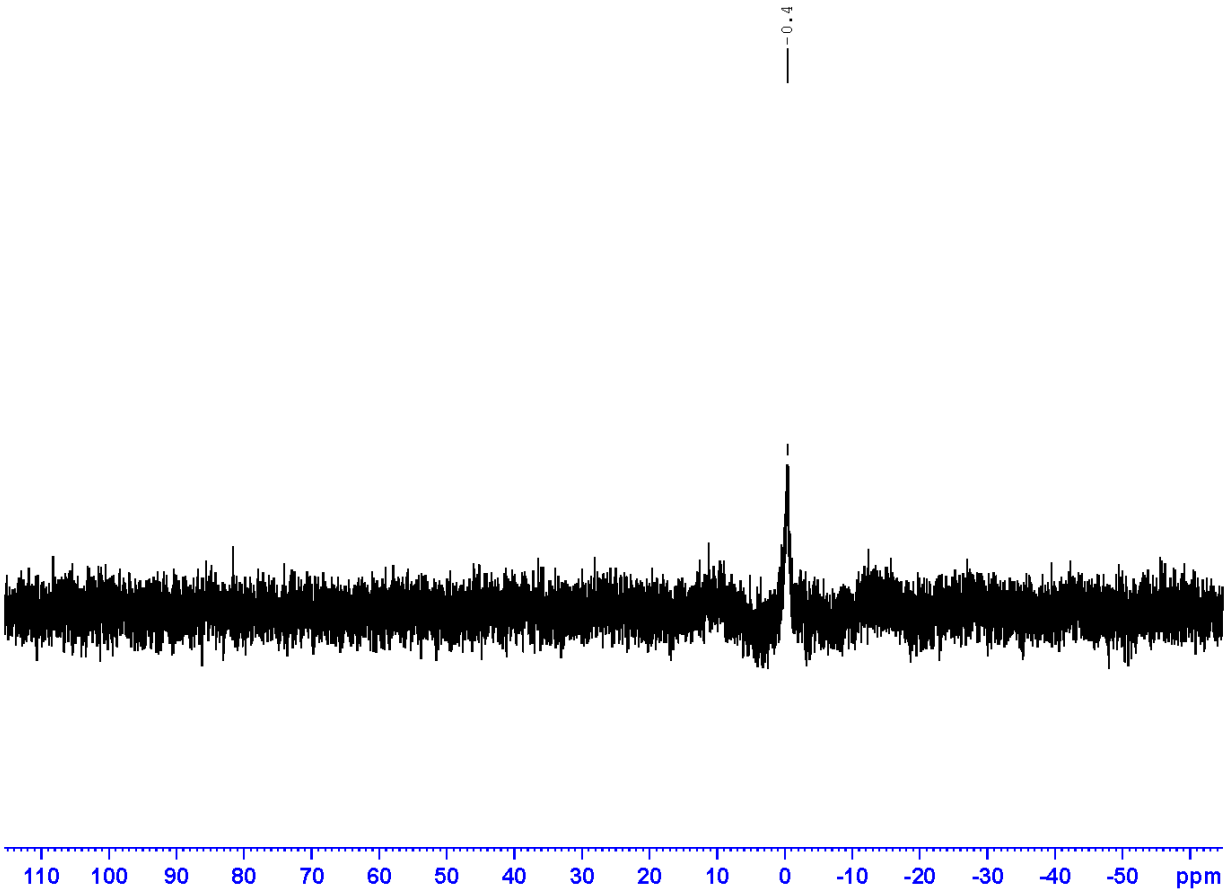
^{13}C NMR (100 MHz, DMSO-d_6)



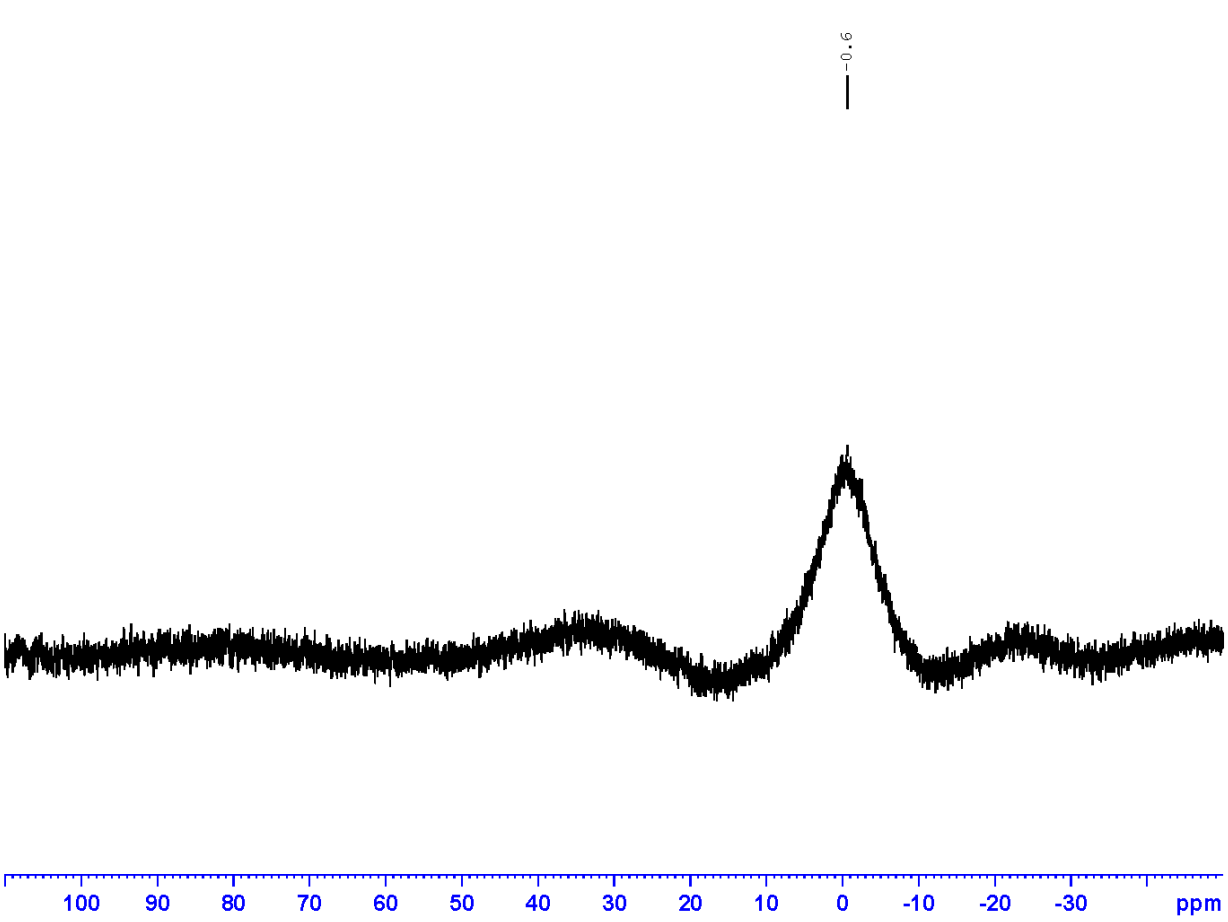
DEPT (100 MHz, DMSO-d_6)



^{11}B NMR (192 MHz, CD_3CN)

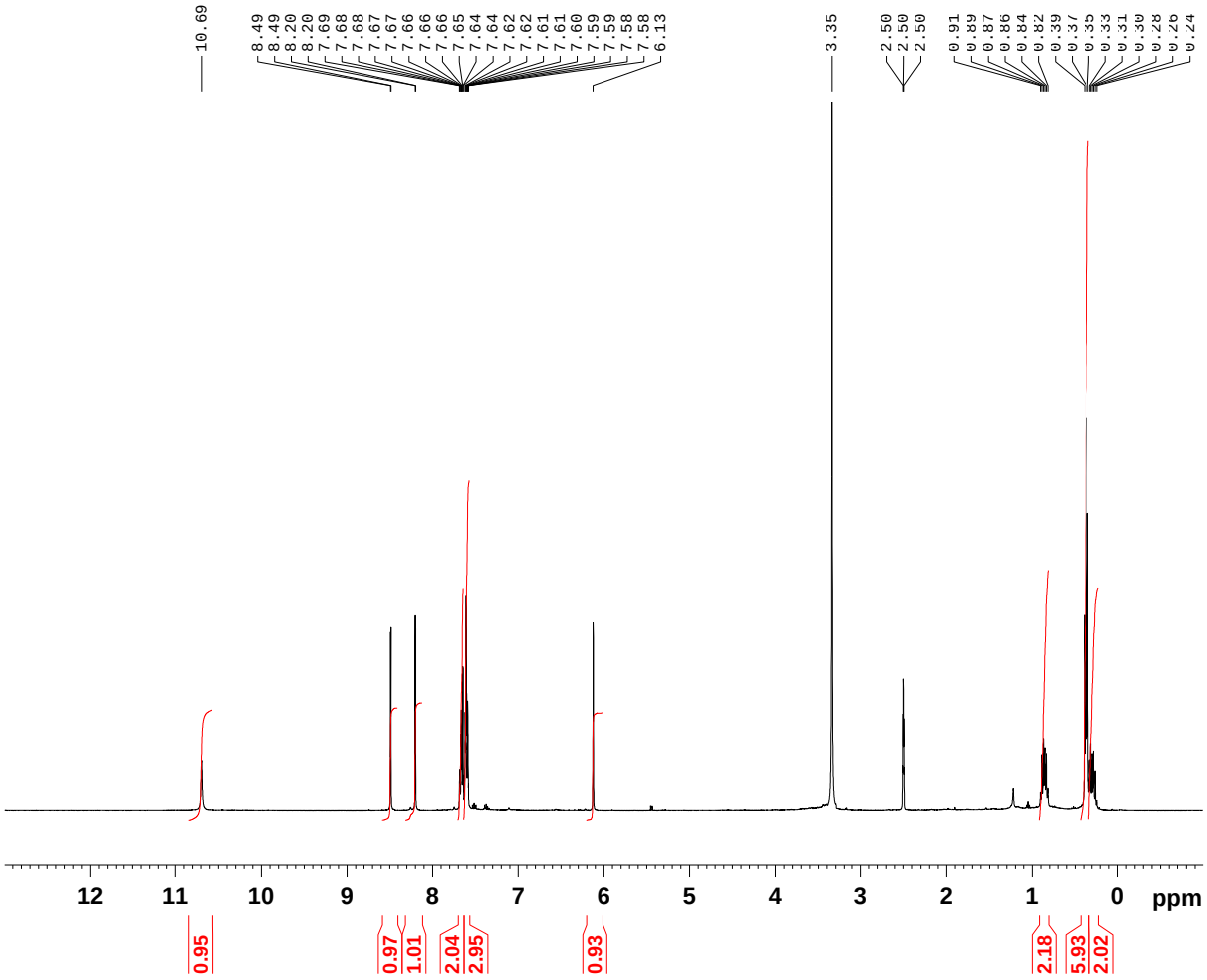


^{11}B NMR (128 MHz, DMSO-d_6)

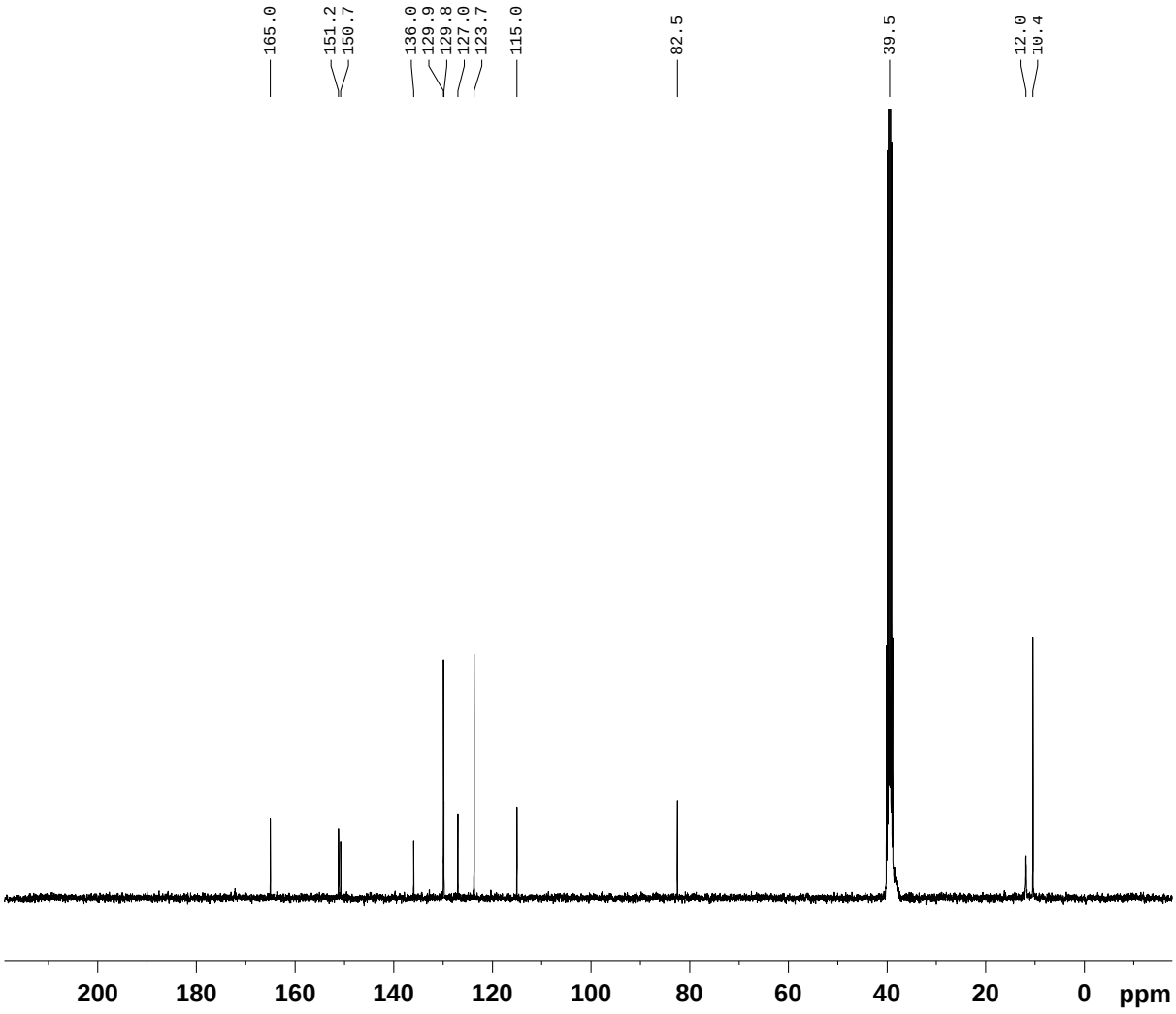


10,10-Diethyl-6,8-dioxo-1-phenyl-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 25c

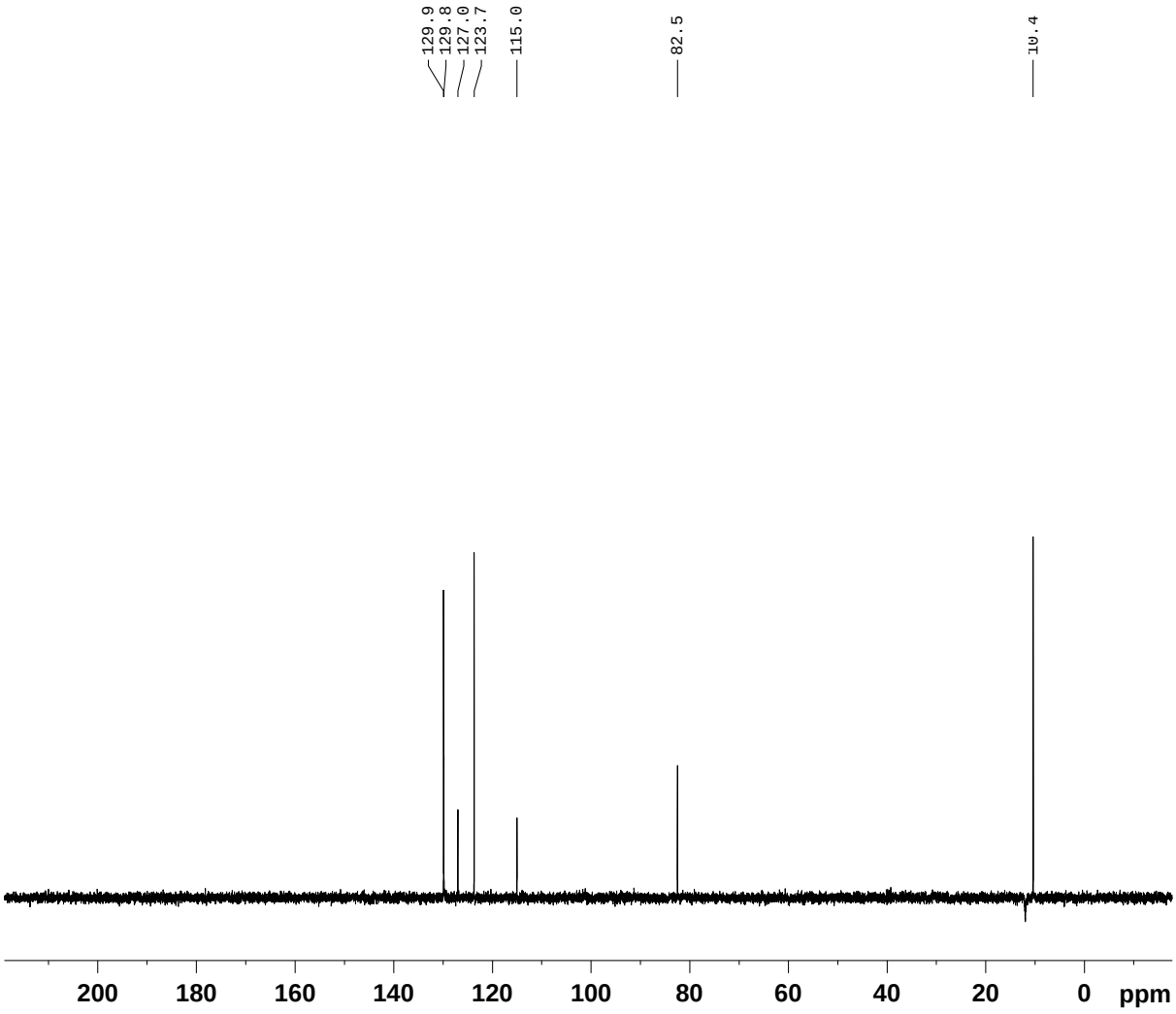
^{1}H NMR (400 MHz, DMSO-d_6)



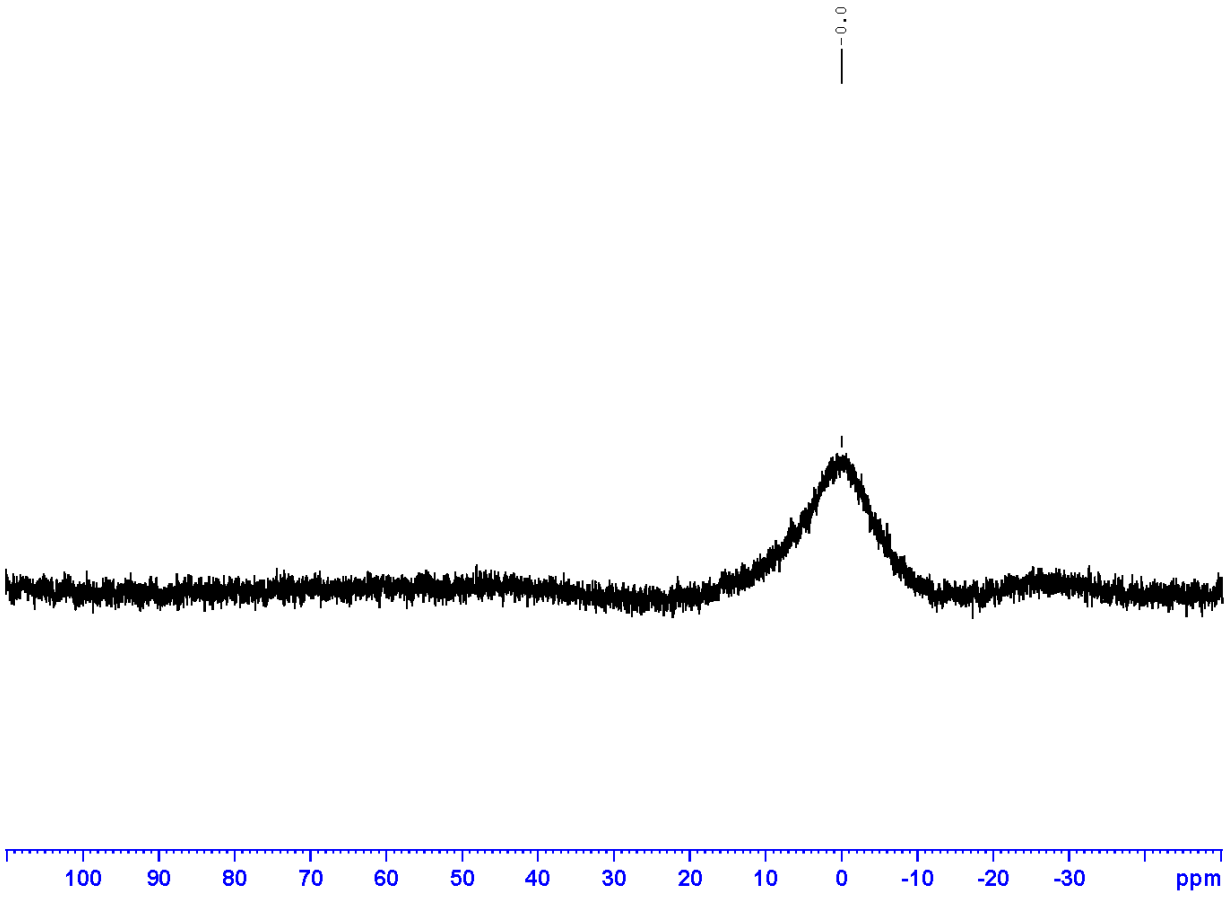
^{13}C NMR (100 MHz, DMSO-d_6)



DEPT (100 MHz, DMSO-d_6)

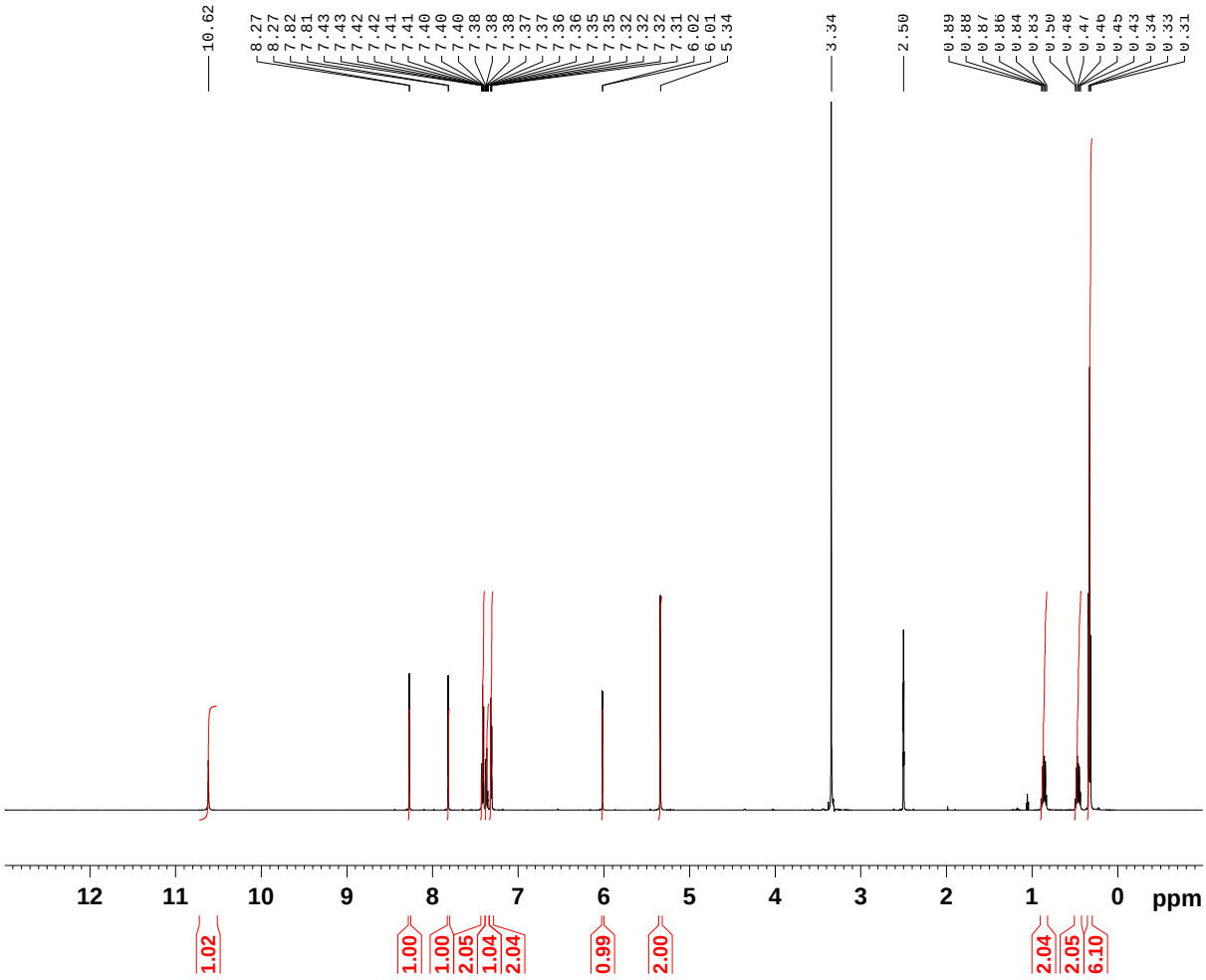


^{11}B NMR (128MHz, DMSO-d_6)

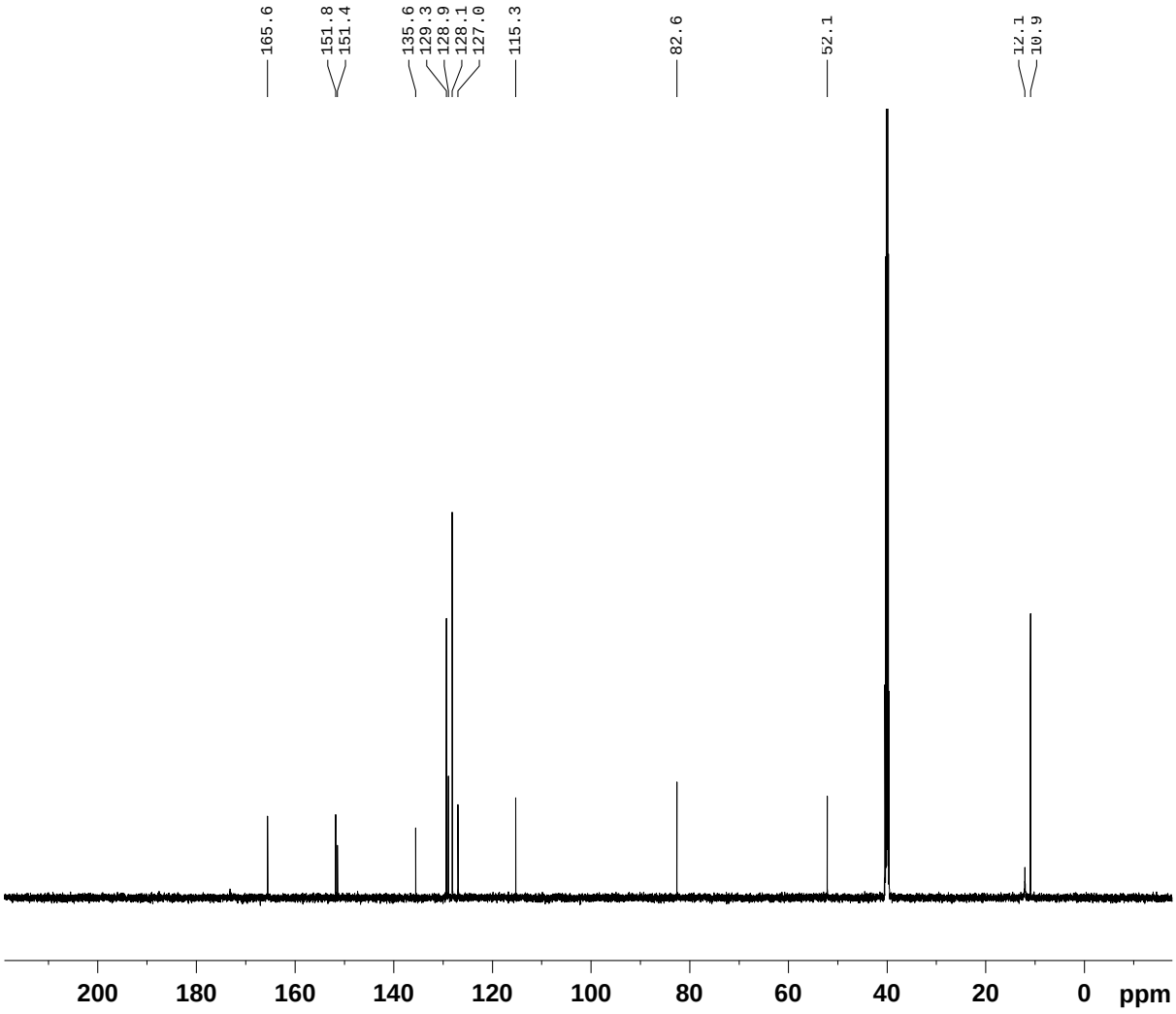


1-Benzyl-10,10-diethyl-6,8-dioxo-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 25d

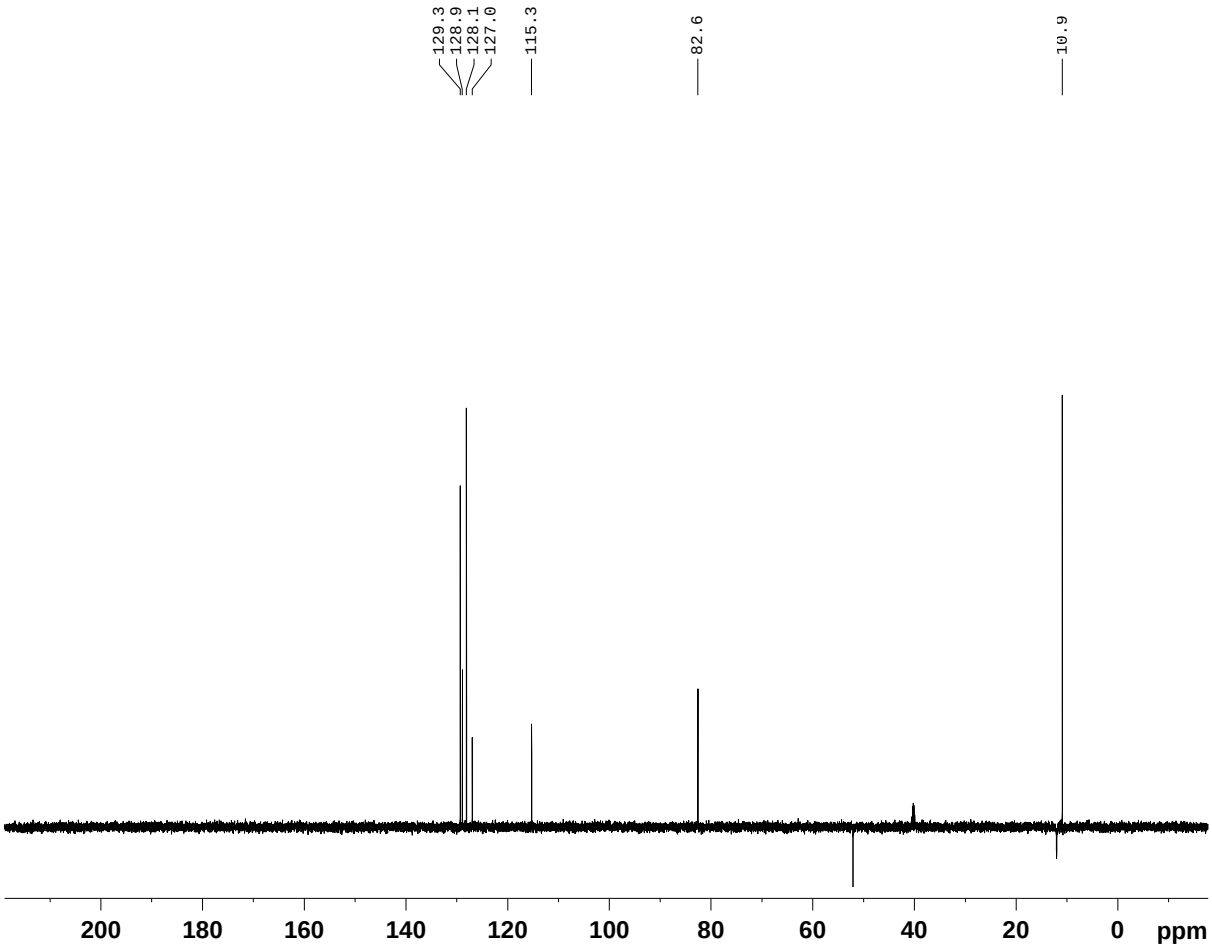
^{1}H NMR (400 MHz, DMSO-d_6)



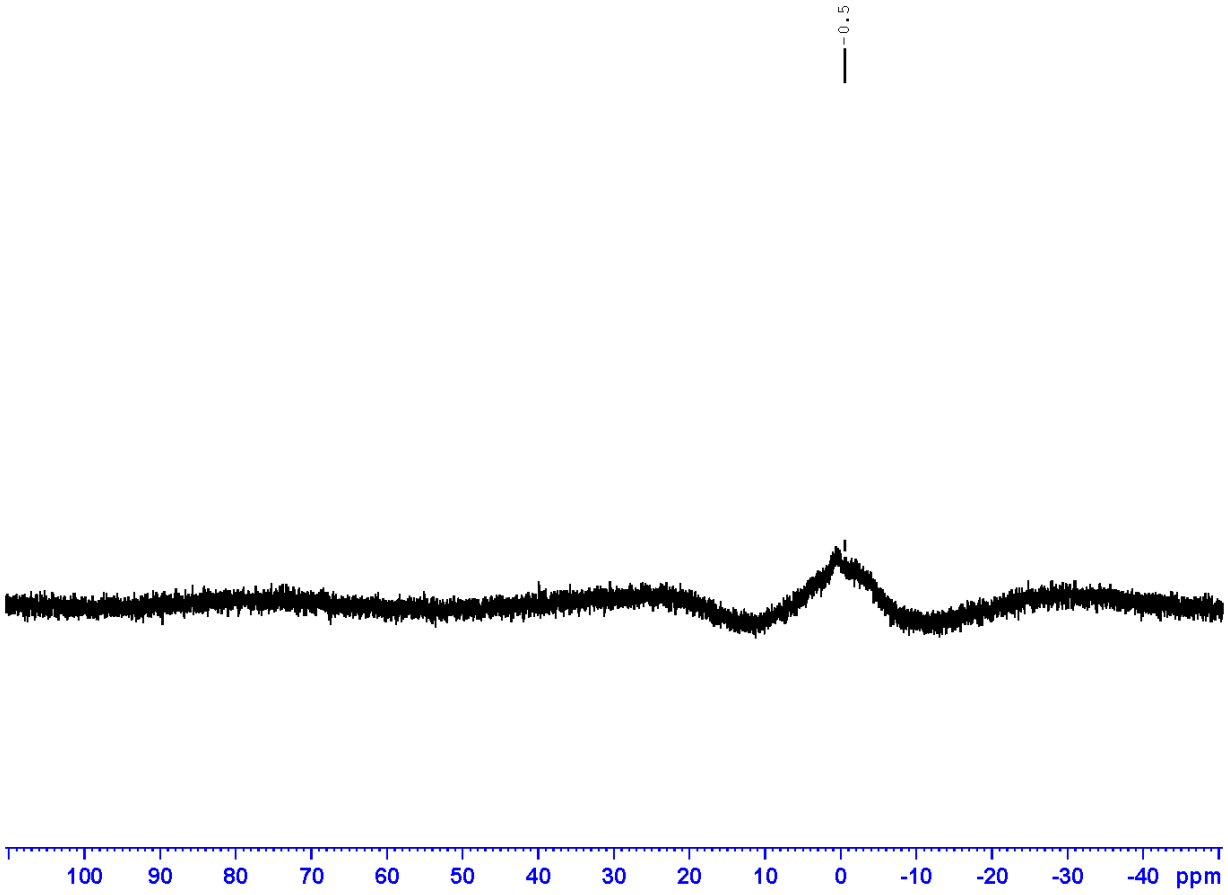
^{13}C NMR (100 MHz, DMSO-d_6)



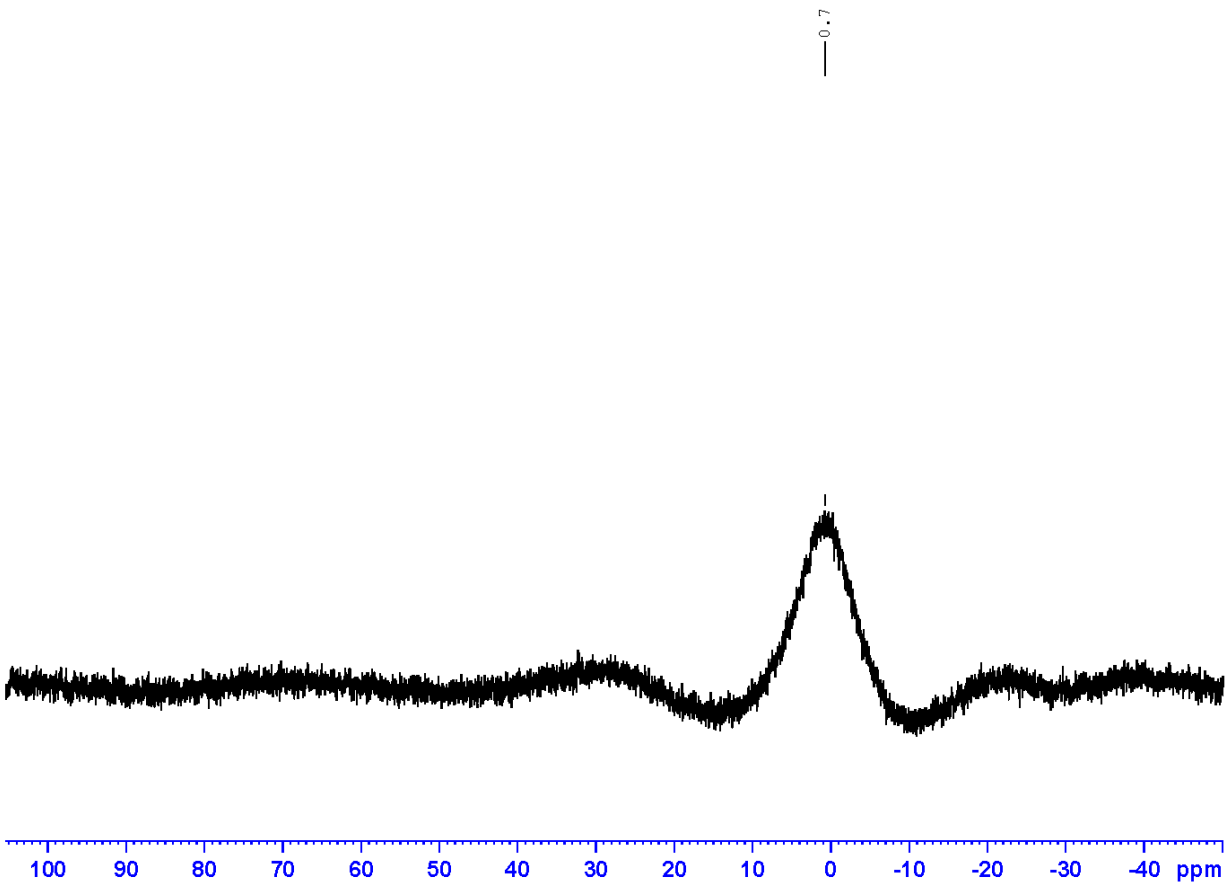
DEPT (100 MHz, DMSO-d_6)



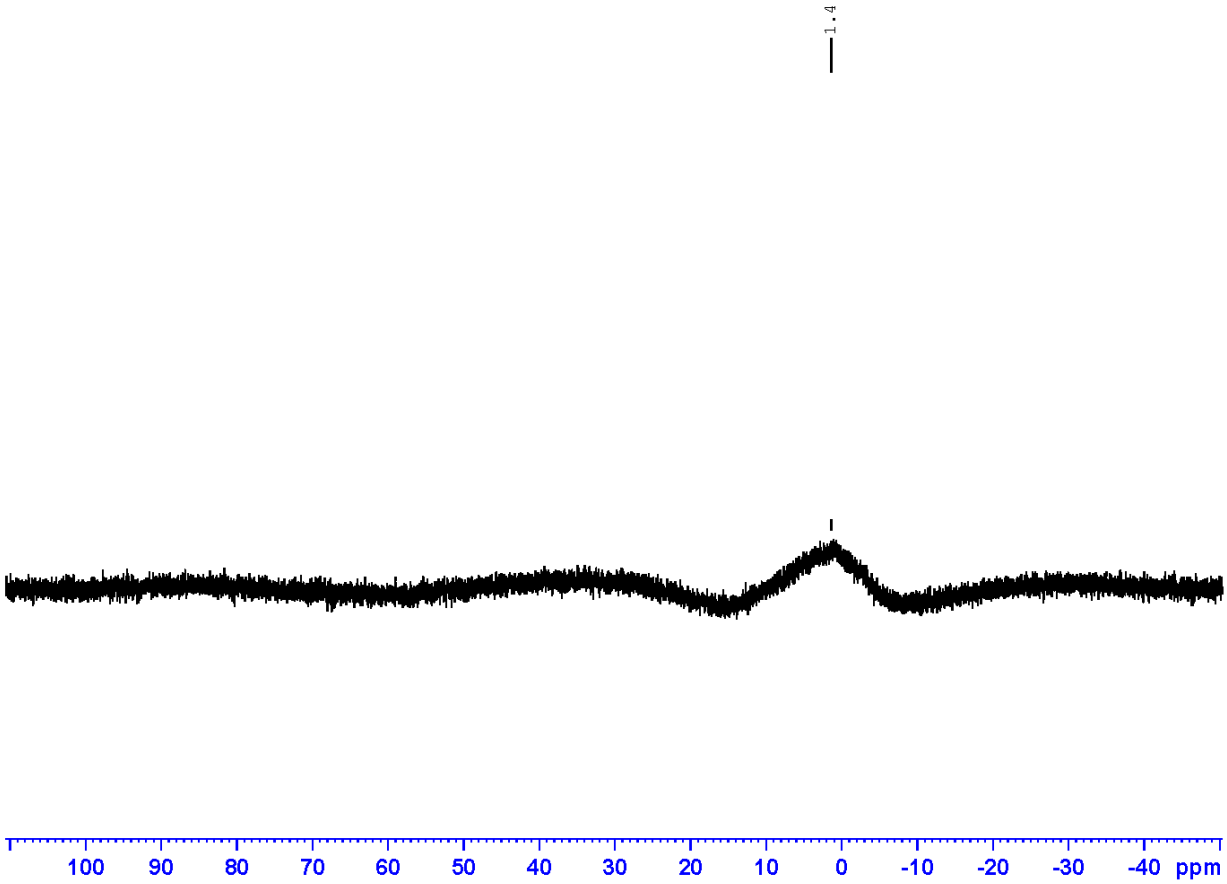
^{11}B NMR (192 MHz, CD_3CN)



^{11}B NMR (128 MHz, DMSO-d_6)

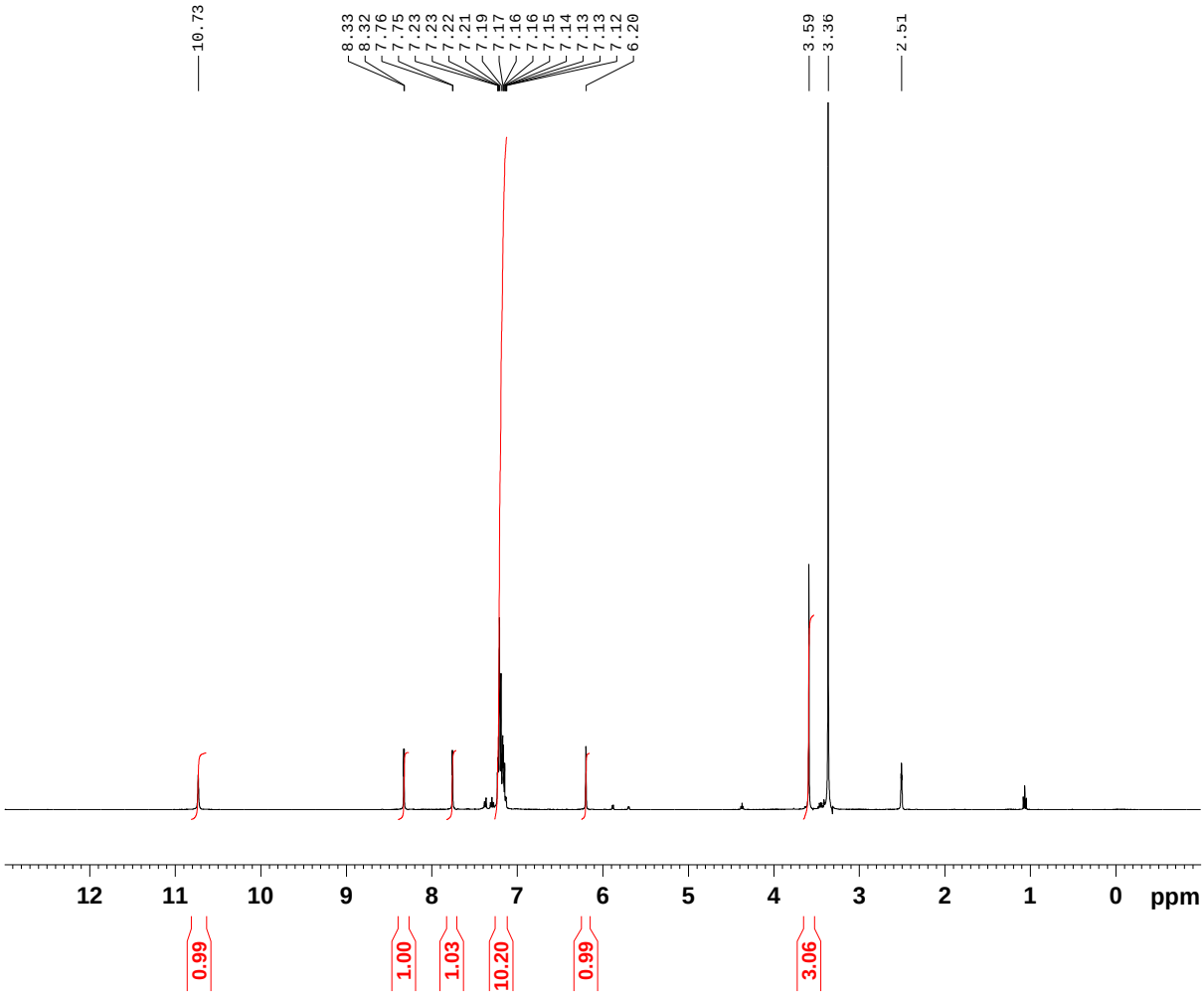


^{11}B NMR (192 MHz, THF-d_8)

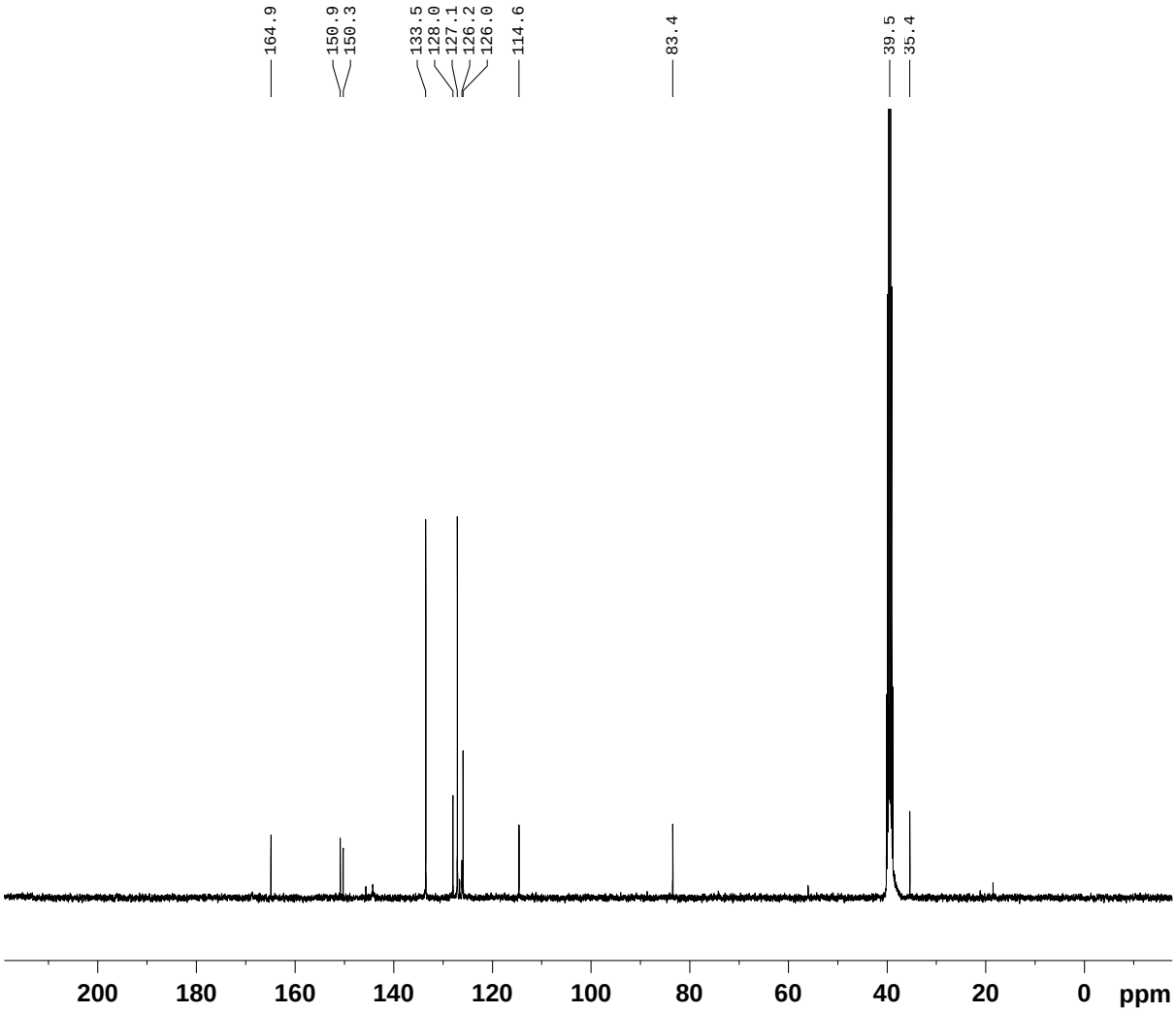


1-Methyl-6,8-dioxo-10,10-diphenyl-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 26a

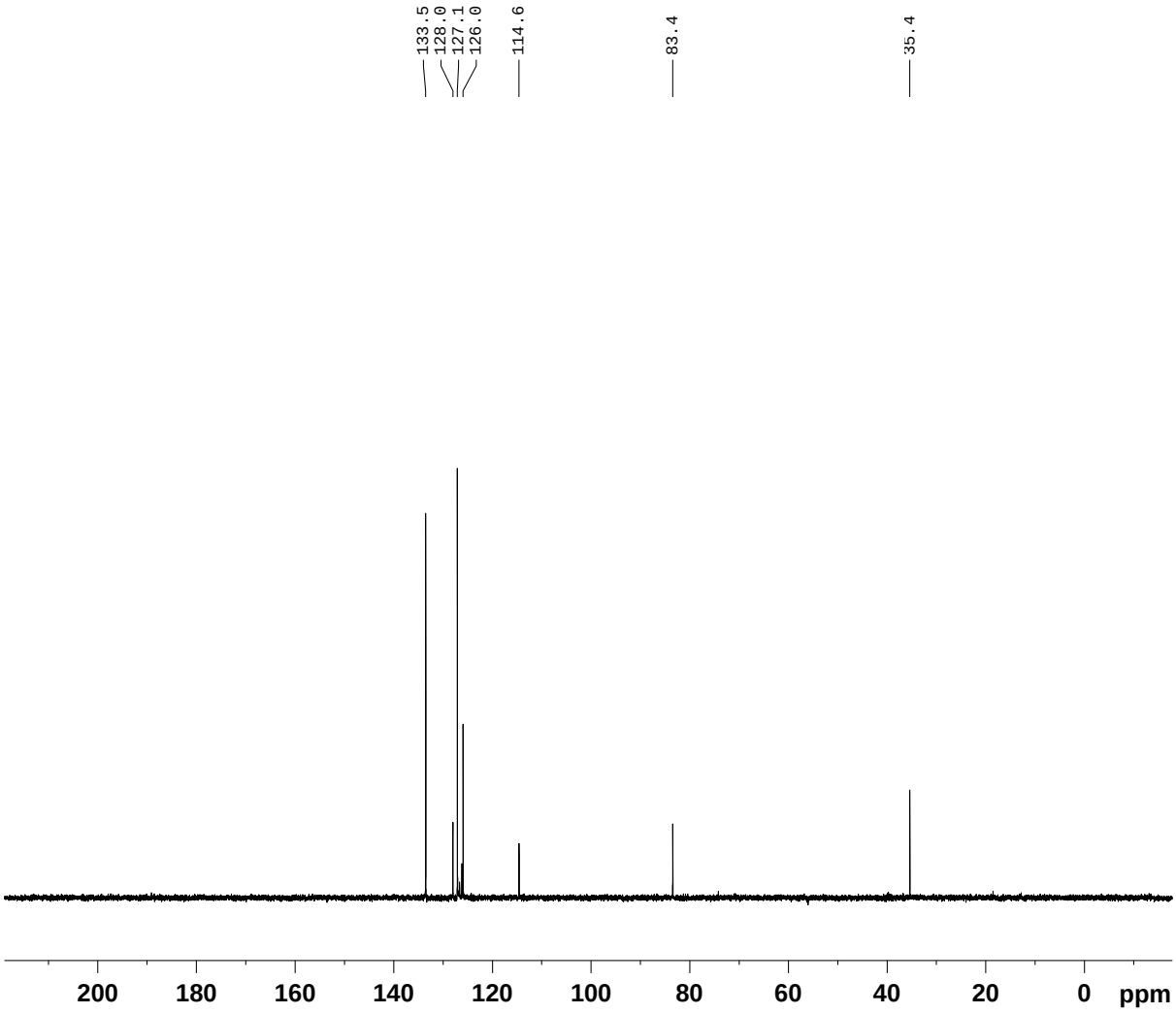
^{1}H NMR (400 MHz, DMSO-d_6)



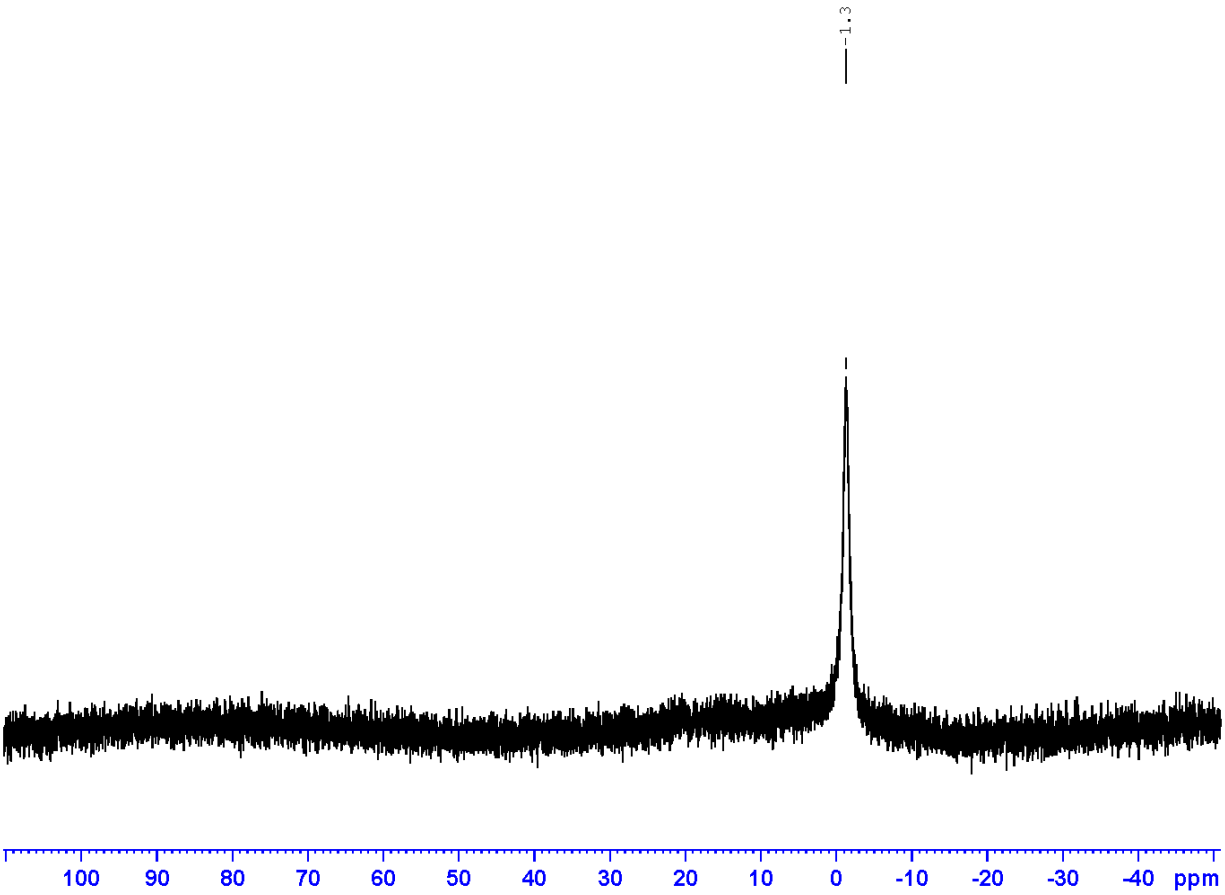
^{13}C NMR (100 MHz, DMSO-d_6)



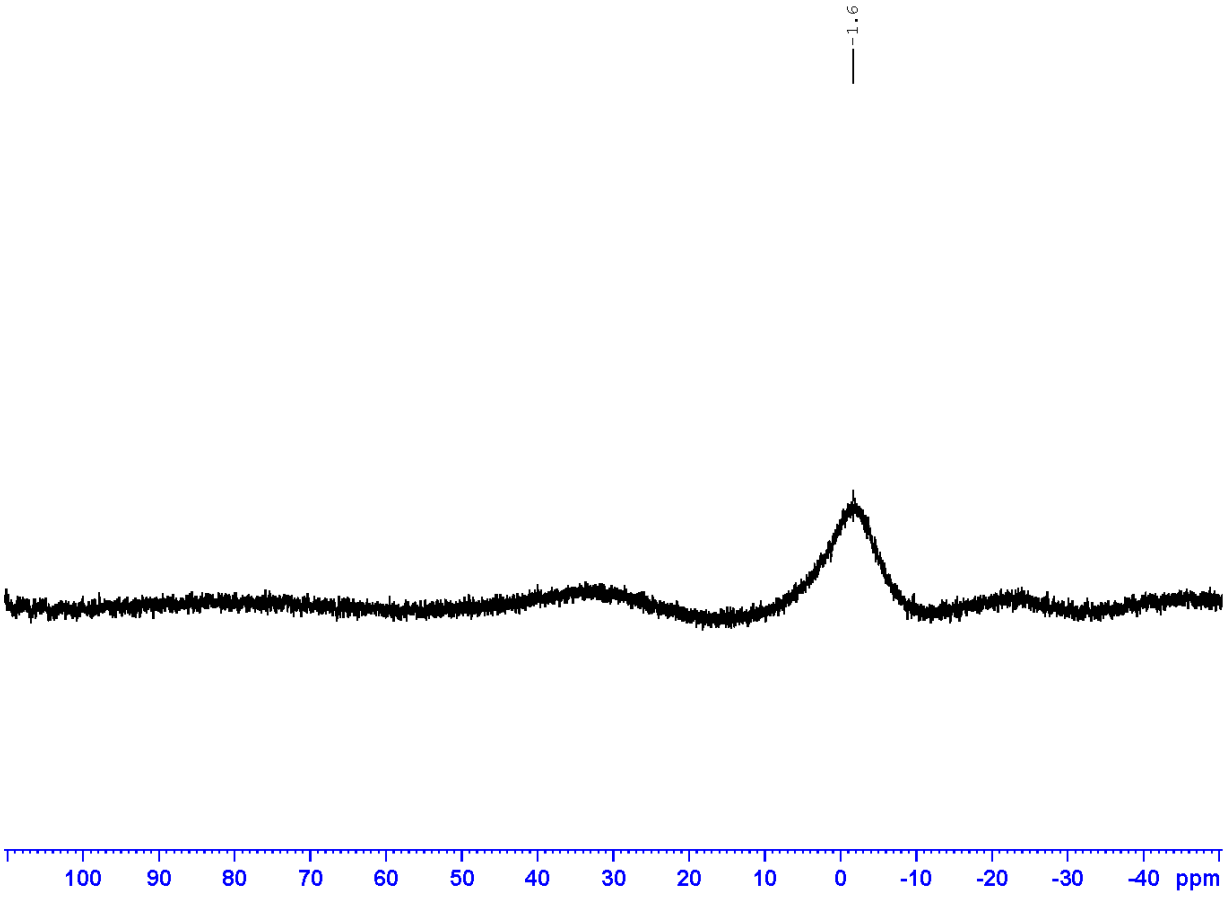
DEPT (100 MHz, DMSO-d_6)



^{11}B NMR (192MHz, CD_3CN)

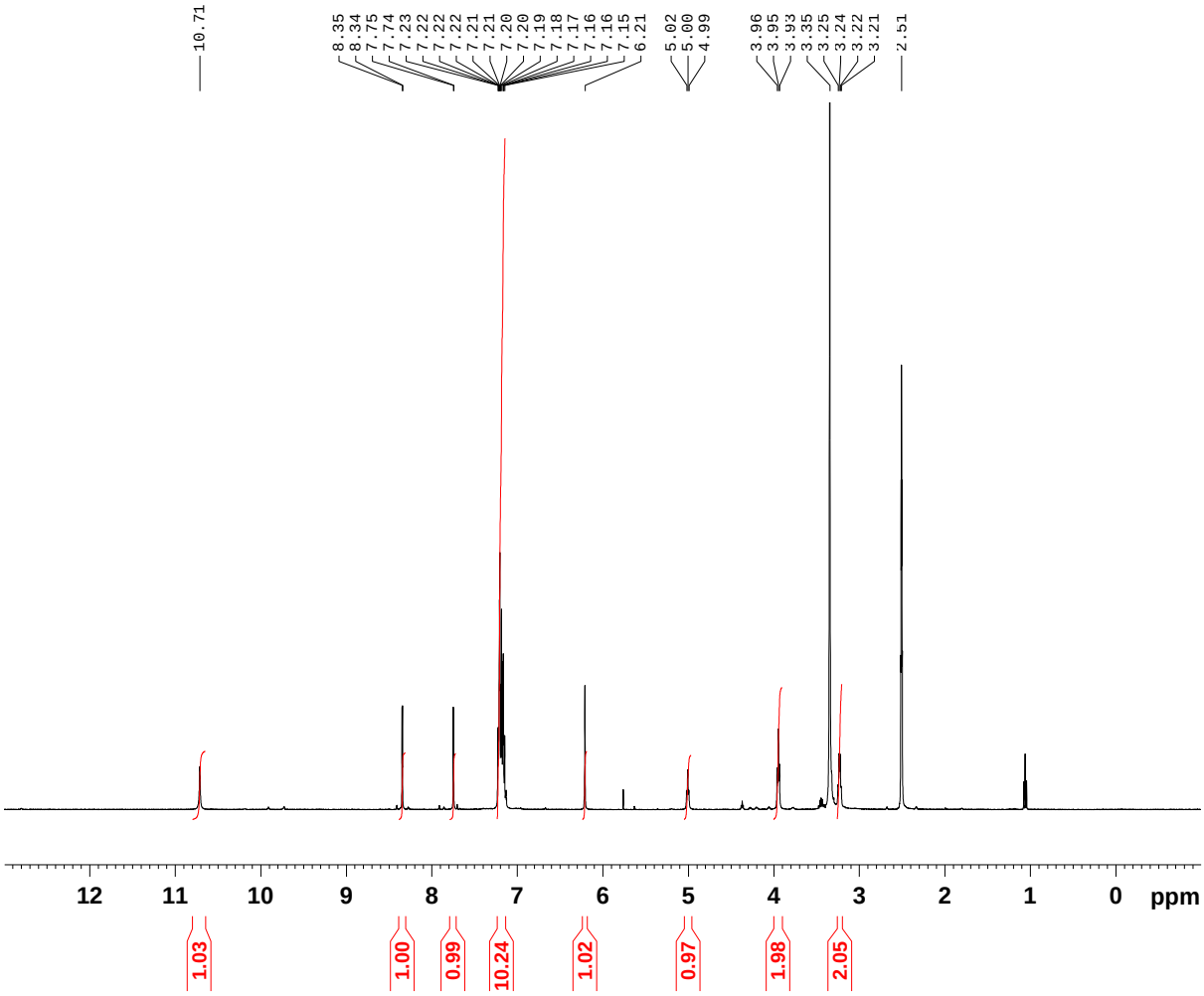


^{11}B NMR (128MHz, DMSO-d_6)

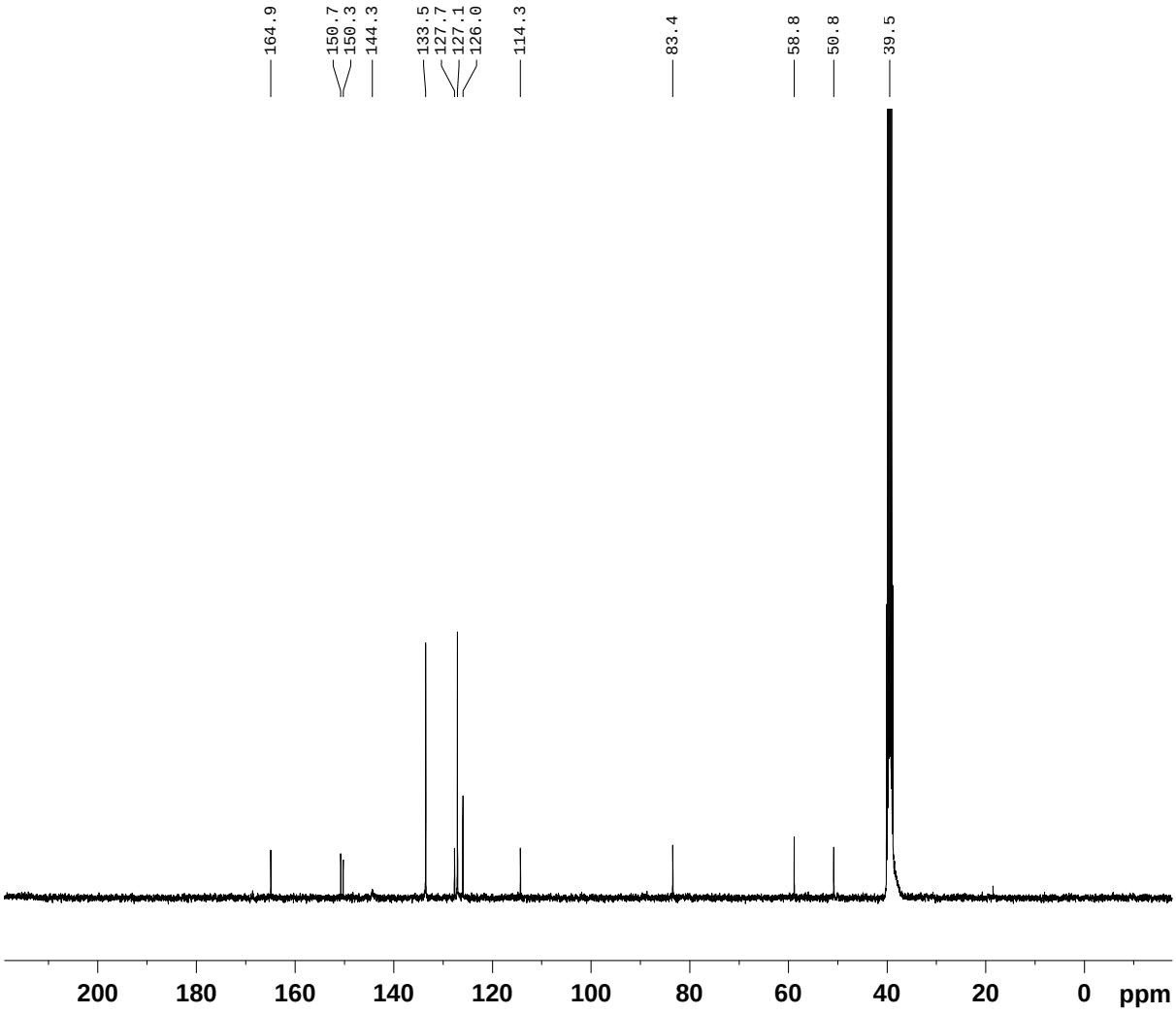


1-(2-Hydroxyethyl)-6,8-dioxo-10,10-diphenyl-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 26b

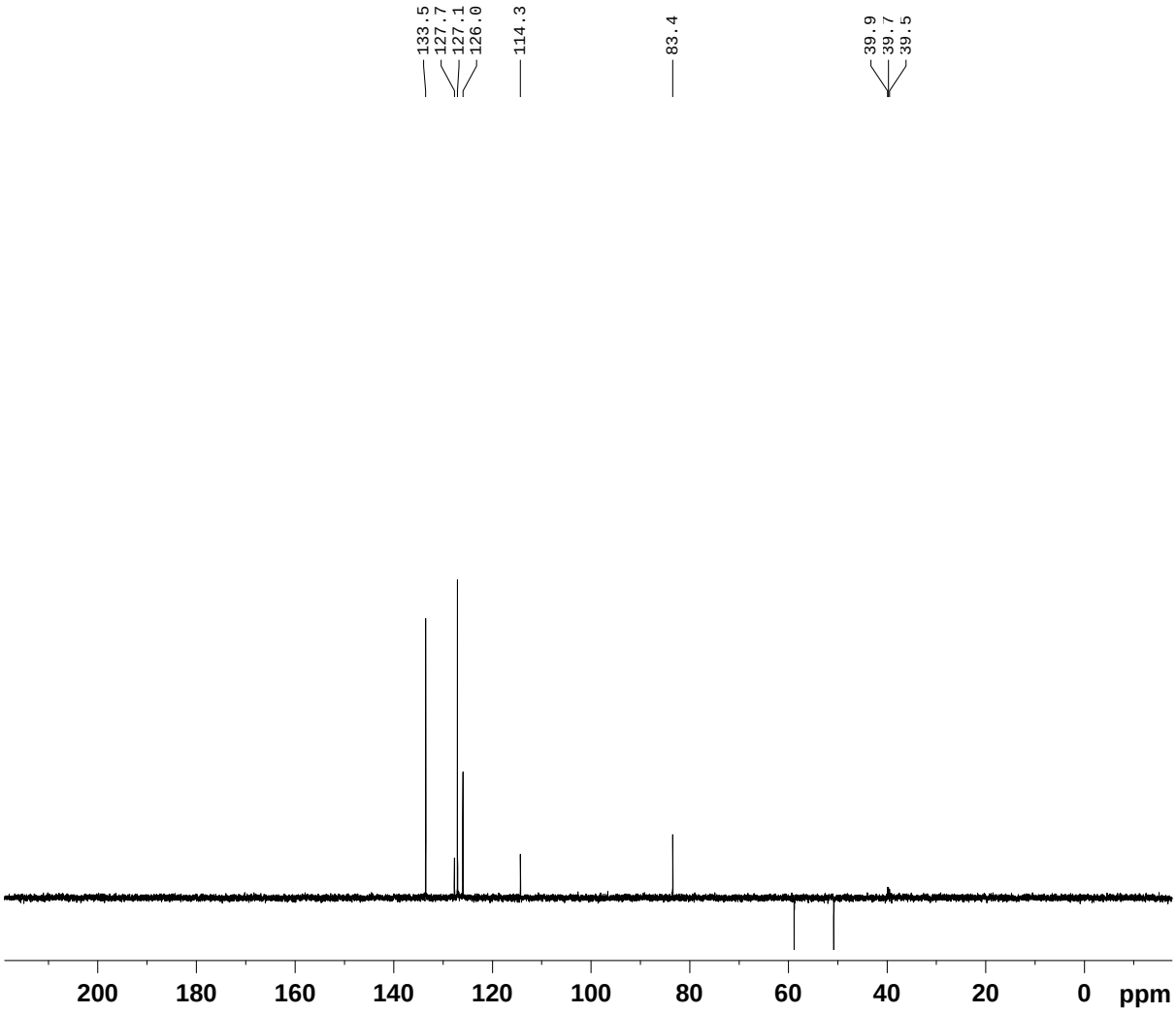
^{1}H NMR (400 MHz, DMSO-d_6)



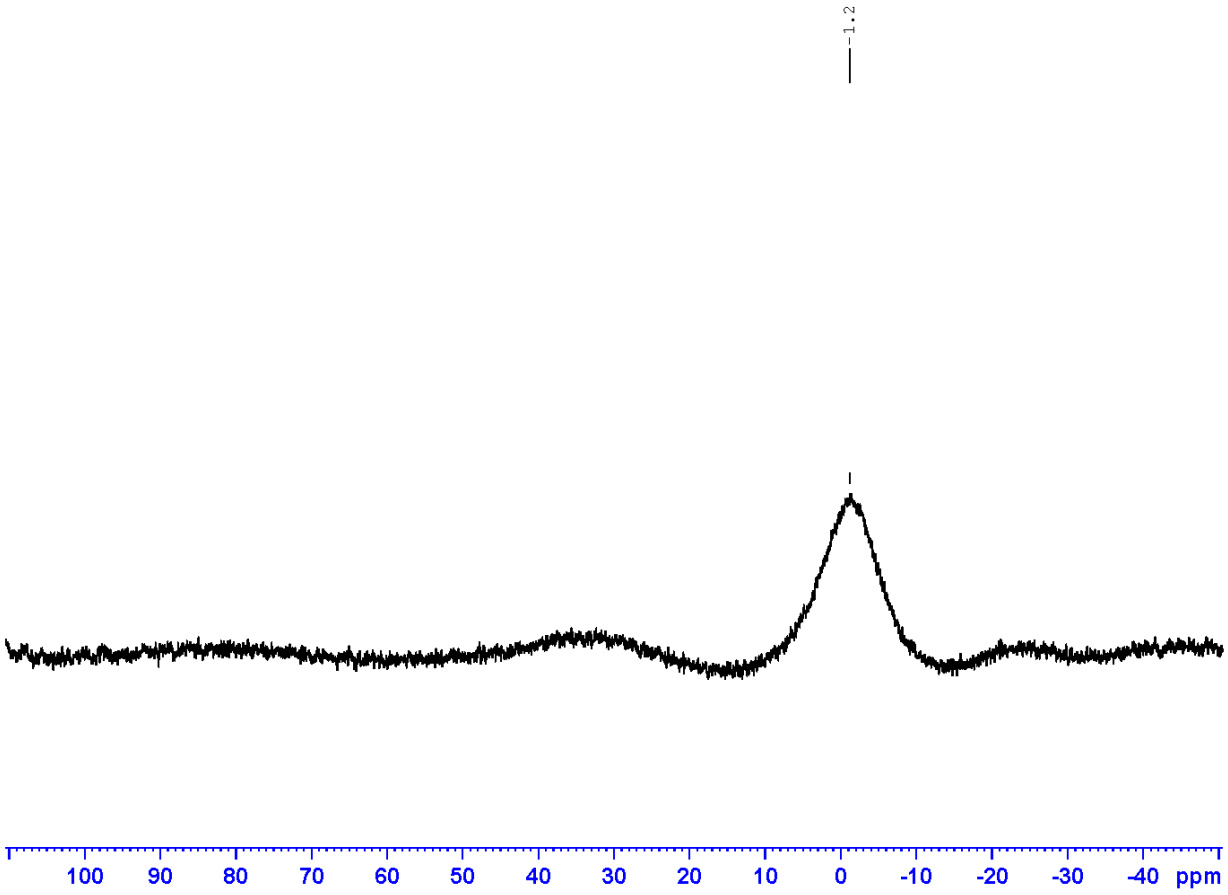
^{13}C NMR (100 MHz, DMSO-d_6)



DEPT (100 MHz, DMSO-d_6)

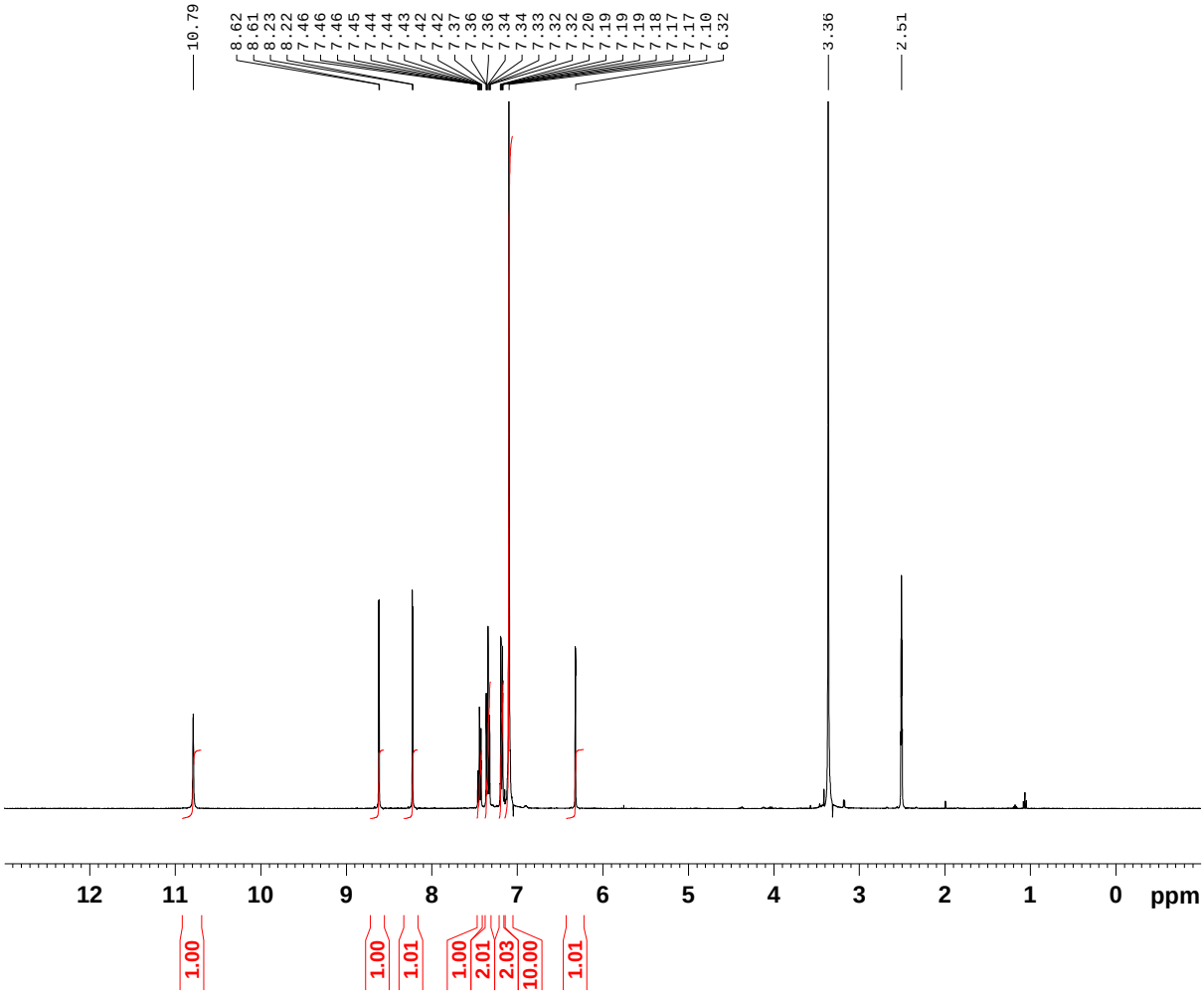


^{11}B NMR (128MHz, DMSO-d_6)

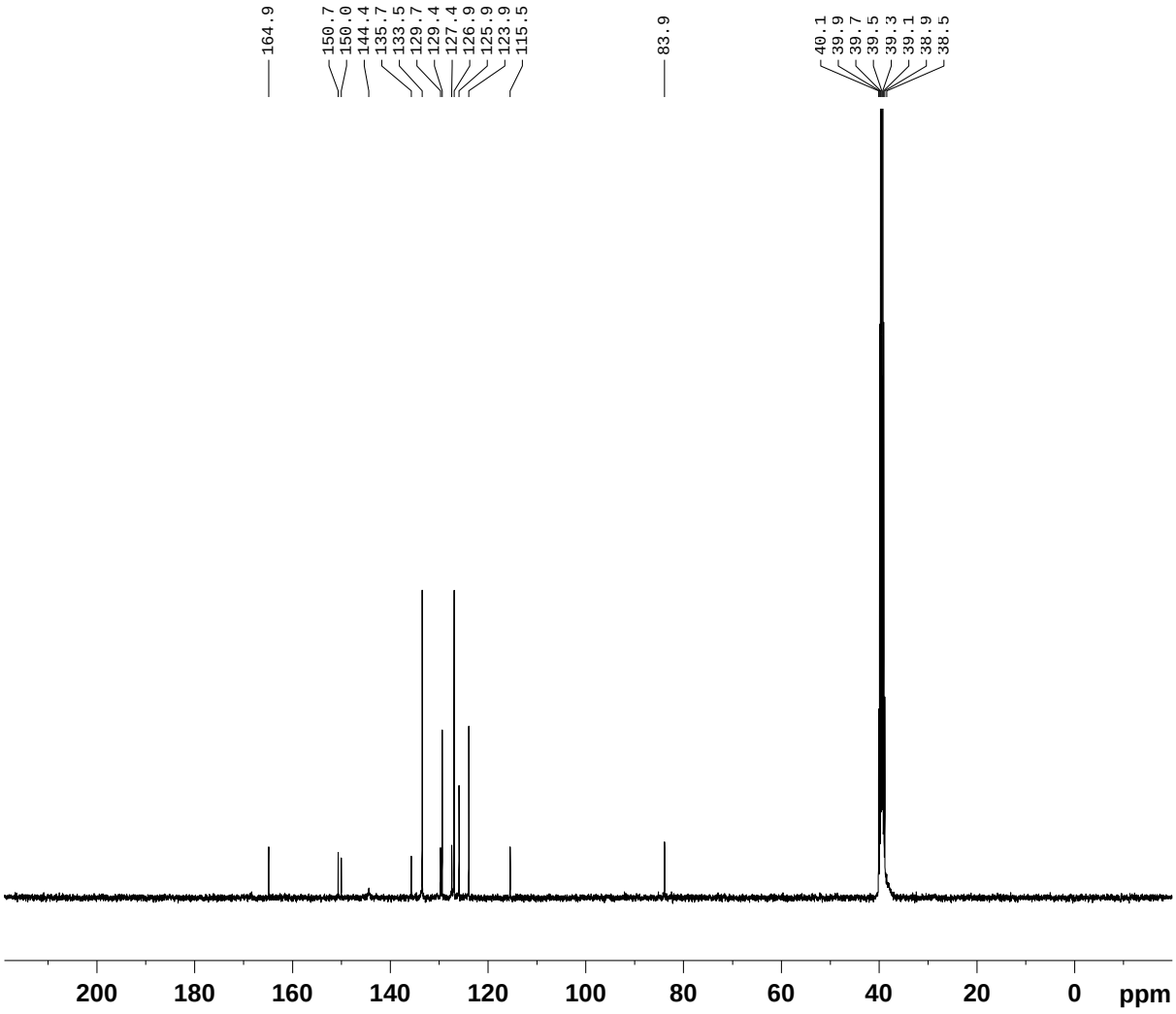


6,8-Dioxo-1,10,10-triphenyl-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 26c

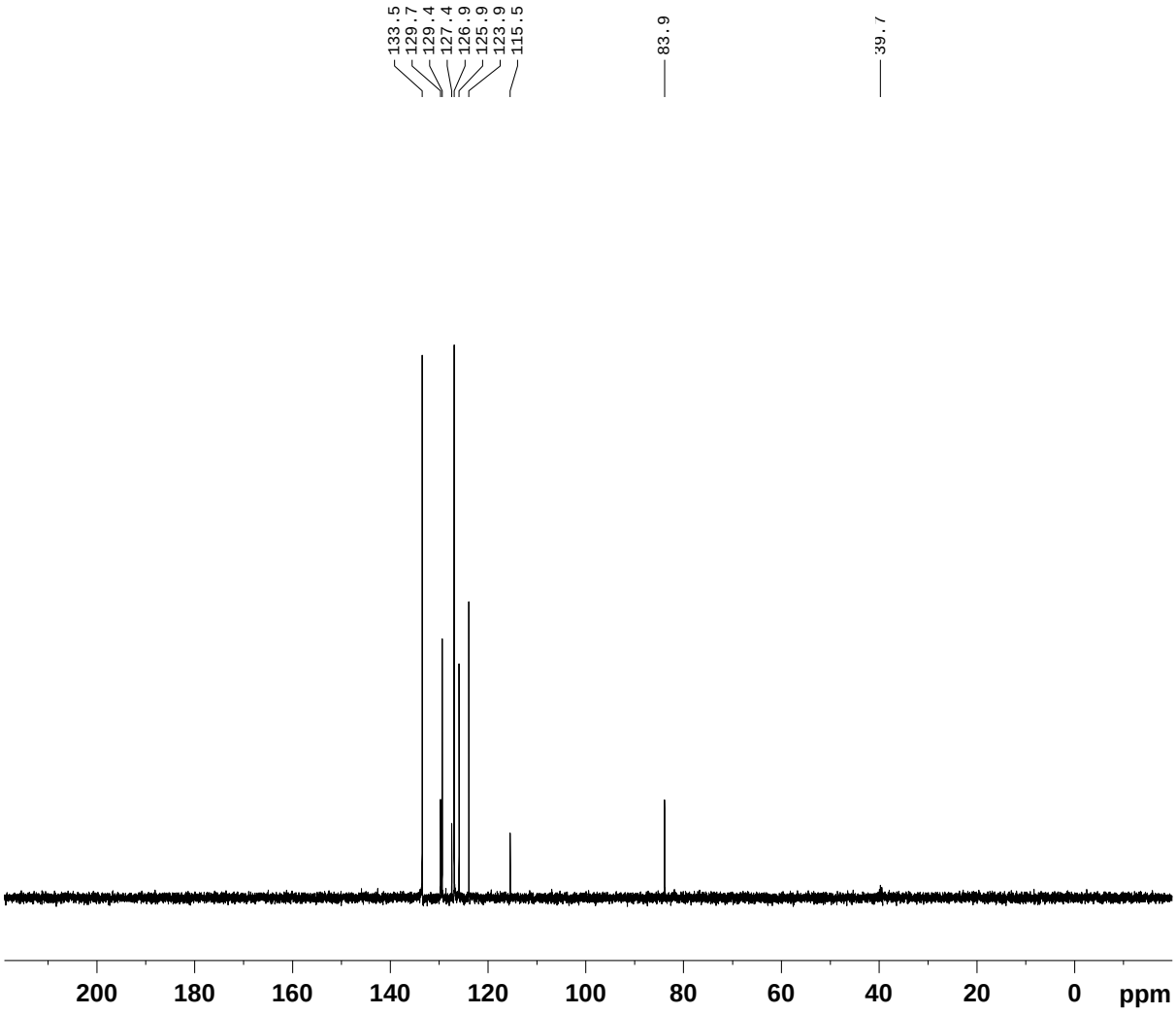
^{1}H NMR (400 MHz, DMSO-d_6)



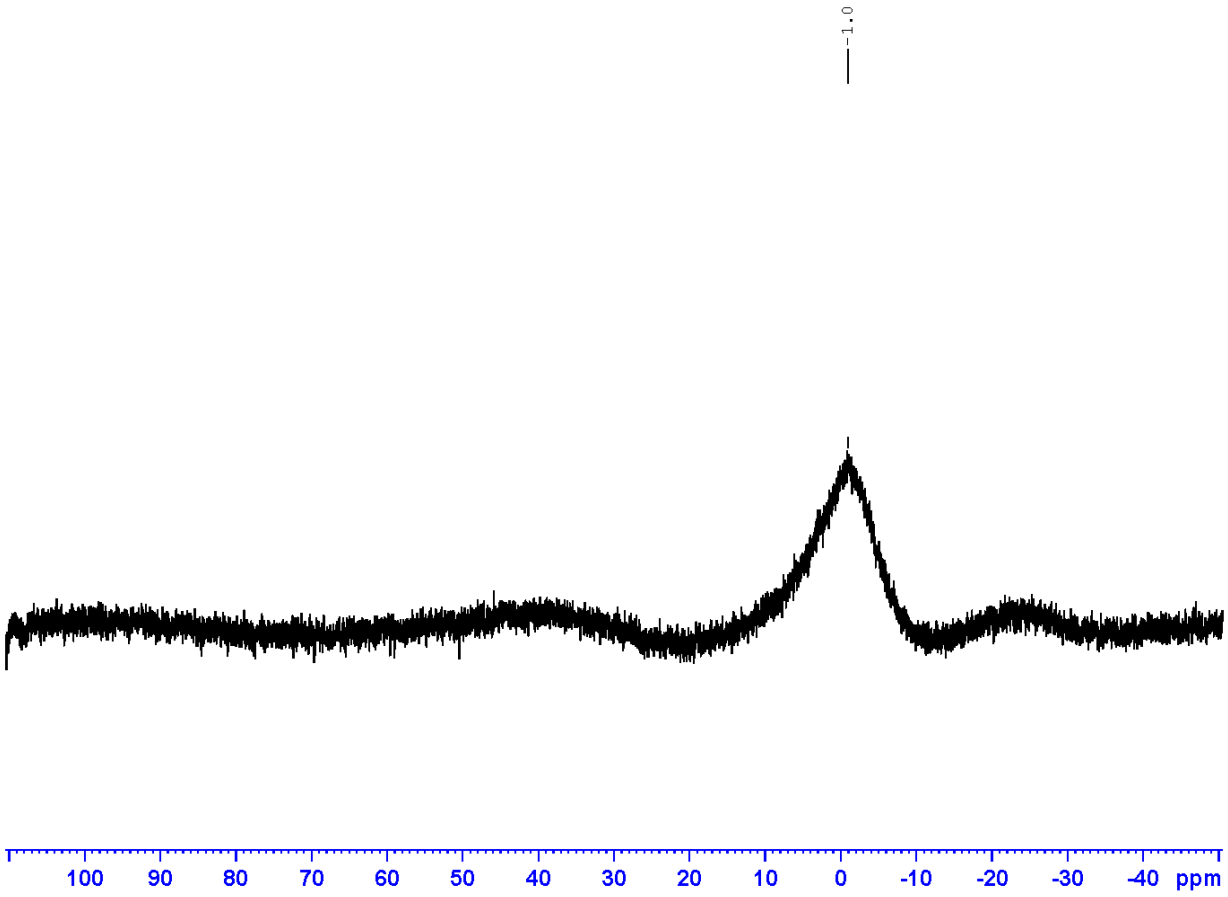
^{13}C NMR (100 MHz, DMSO-d_6)



DEPT (100 MHz, DMSO-d_6)

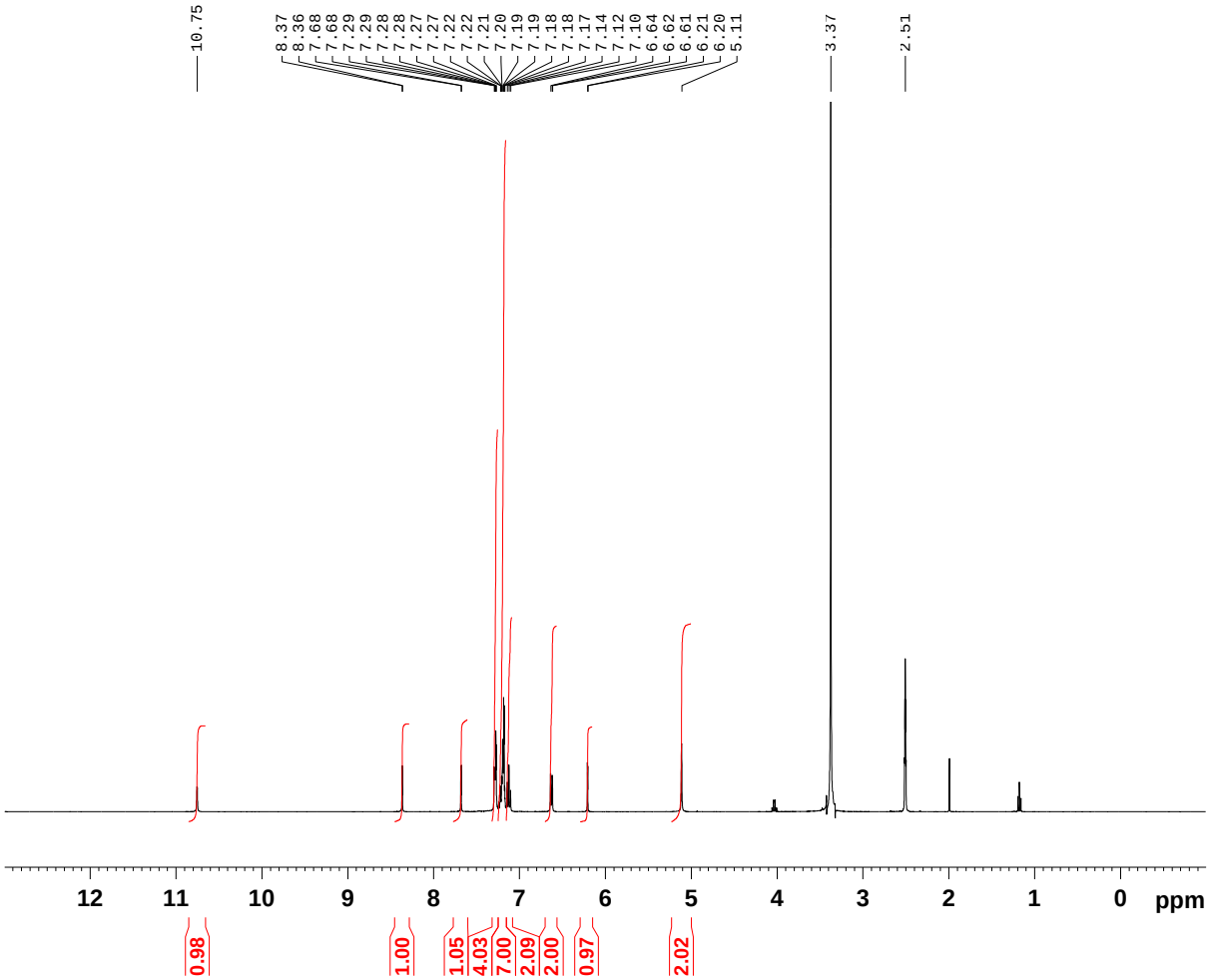


^{11}B NMR (128MHz, DMSO-d_6)

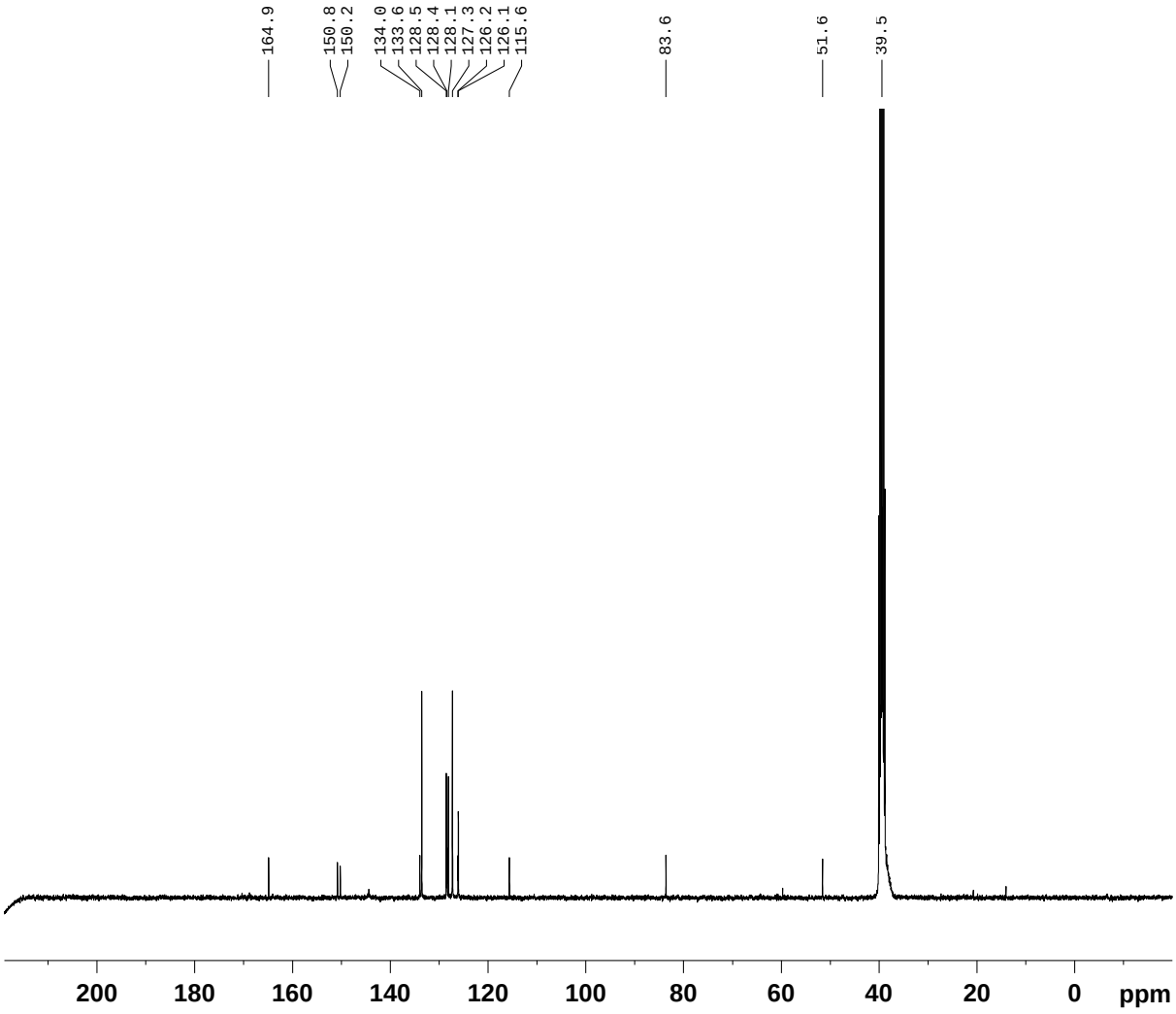


1-Benzyl-6,8-dioxo-10,10-diphenyl-6,7,8,10-tetrahydro-1*H*-imidazo[2',1':3,4][1,4,2]diazaborolo[1,5-c]pyrimidin-4-ium-10-ide 26d

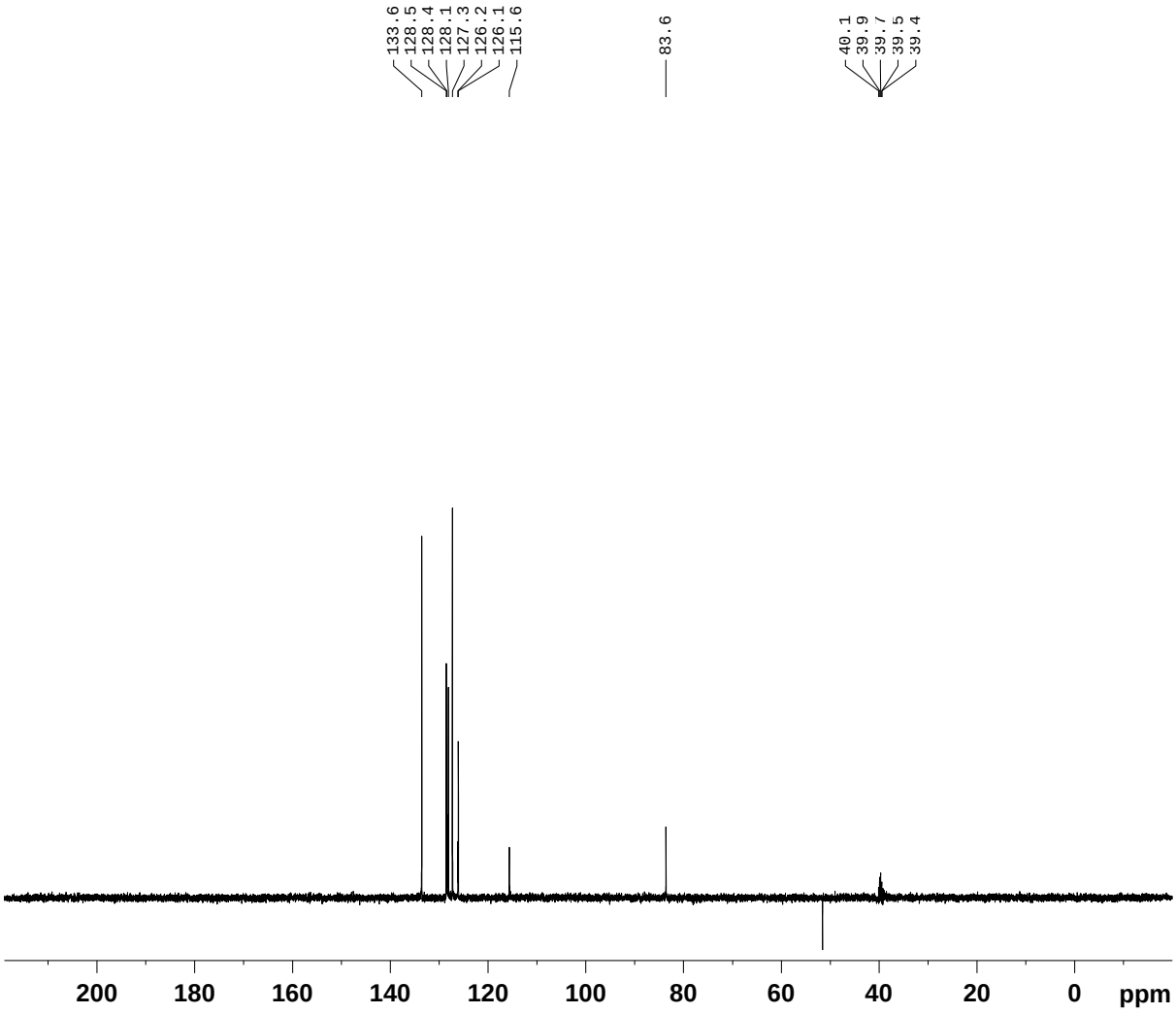
^{1}H NMR (400 MHz, DMSO-d_6)



^{13}C NMR (100 MHz, DMSO-d_6)



DEPT (100 MHz, DMSO-d_6)



^{11}B NMR (128MHz, DMSO-d_6)