Supporting Information

for

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF DIAZULENYLBORINIC ACID

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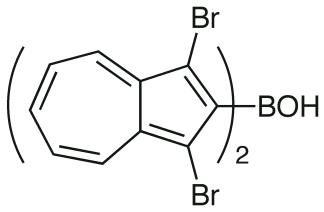
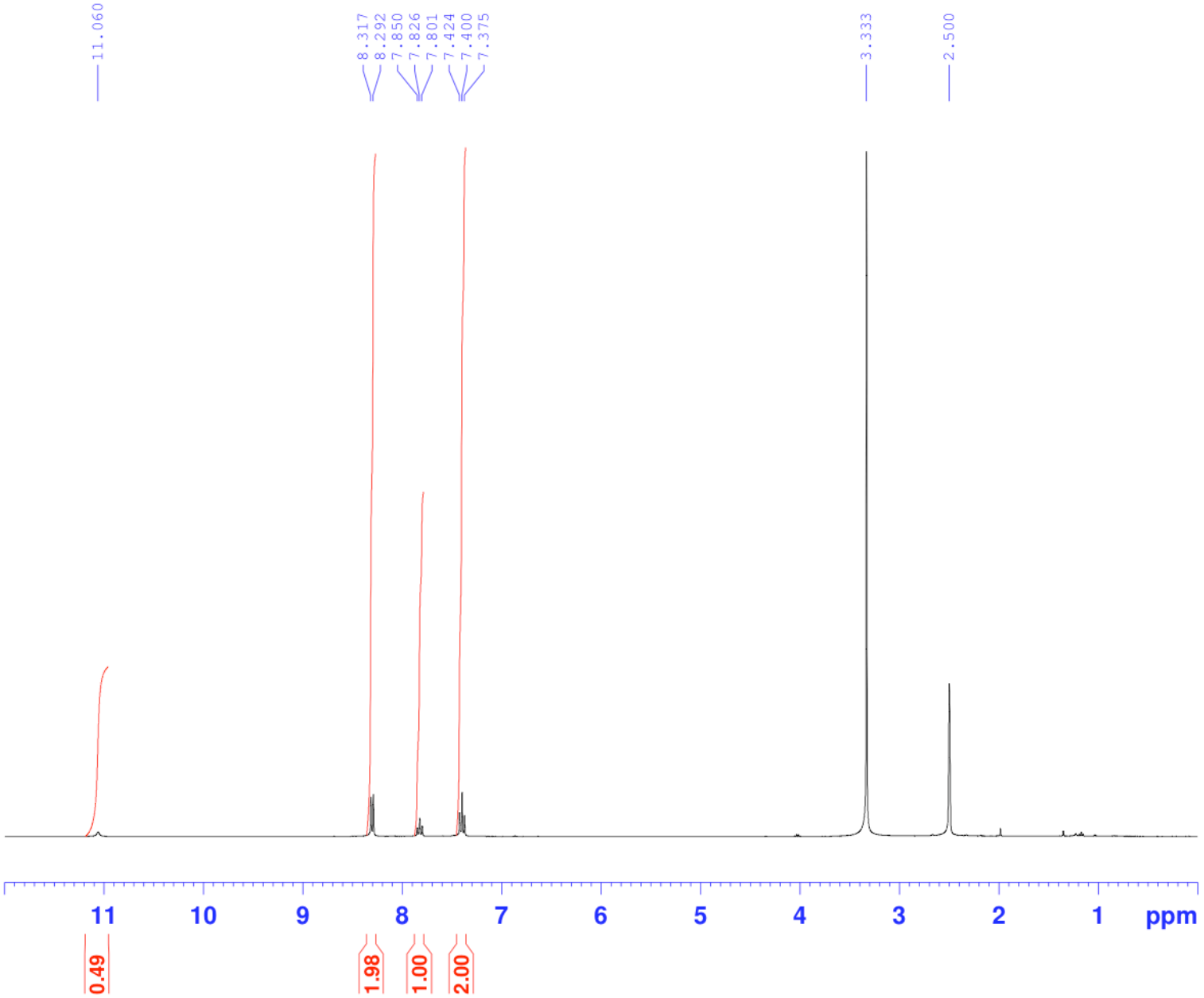
Contents

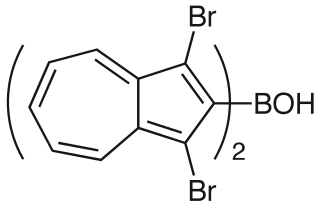


1

^{1}H NMR

(400 MHz, DMSO-d_6)





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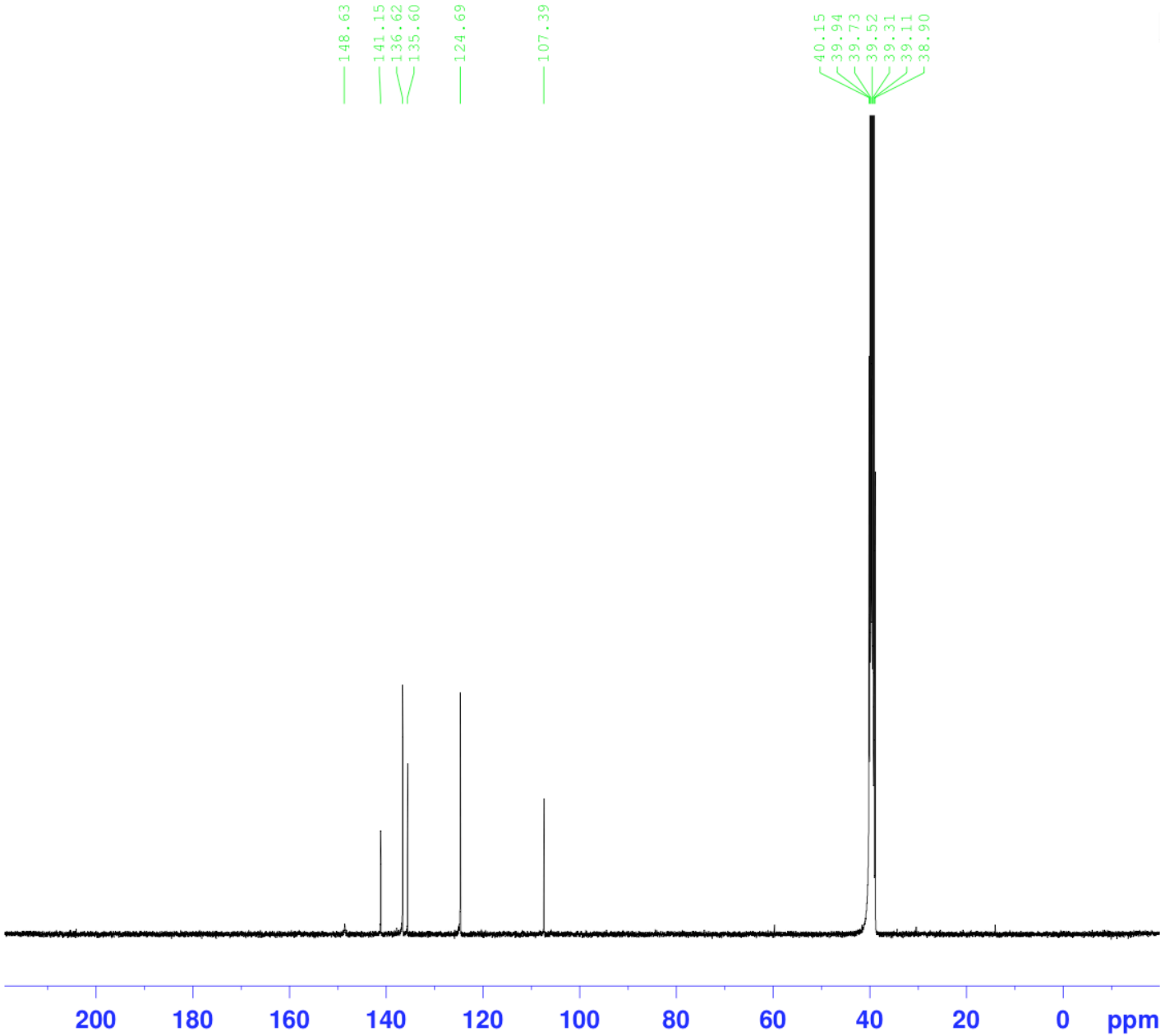
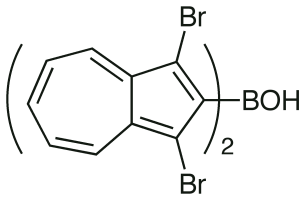
^{13}C NMR

(100 MHz, DMSO-d_6)

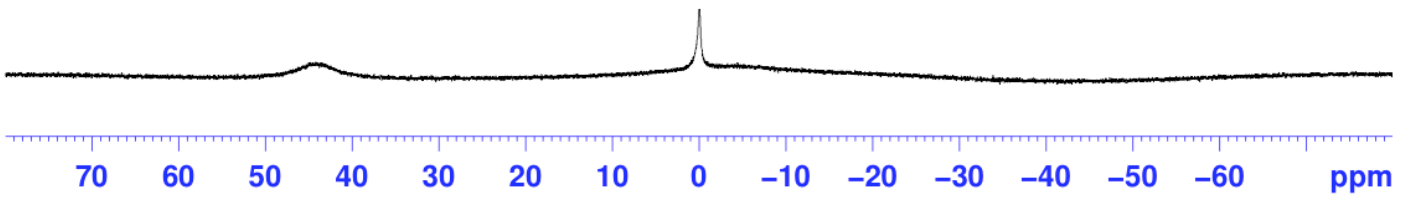


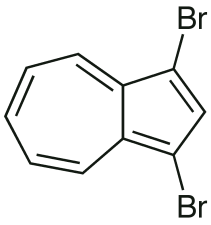


1

^{11}B NMR

(128 MHz, THF-d_8)





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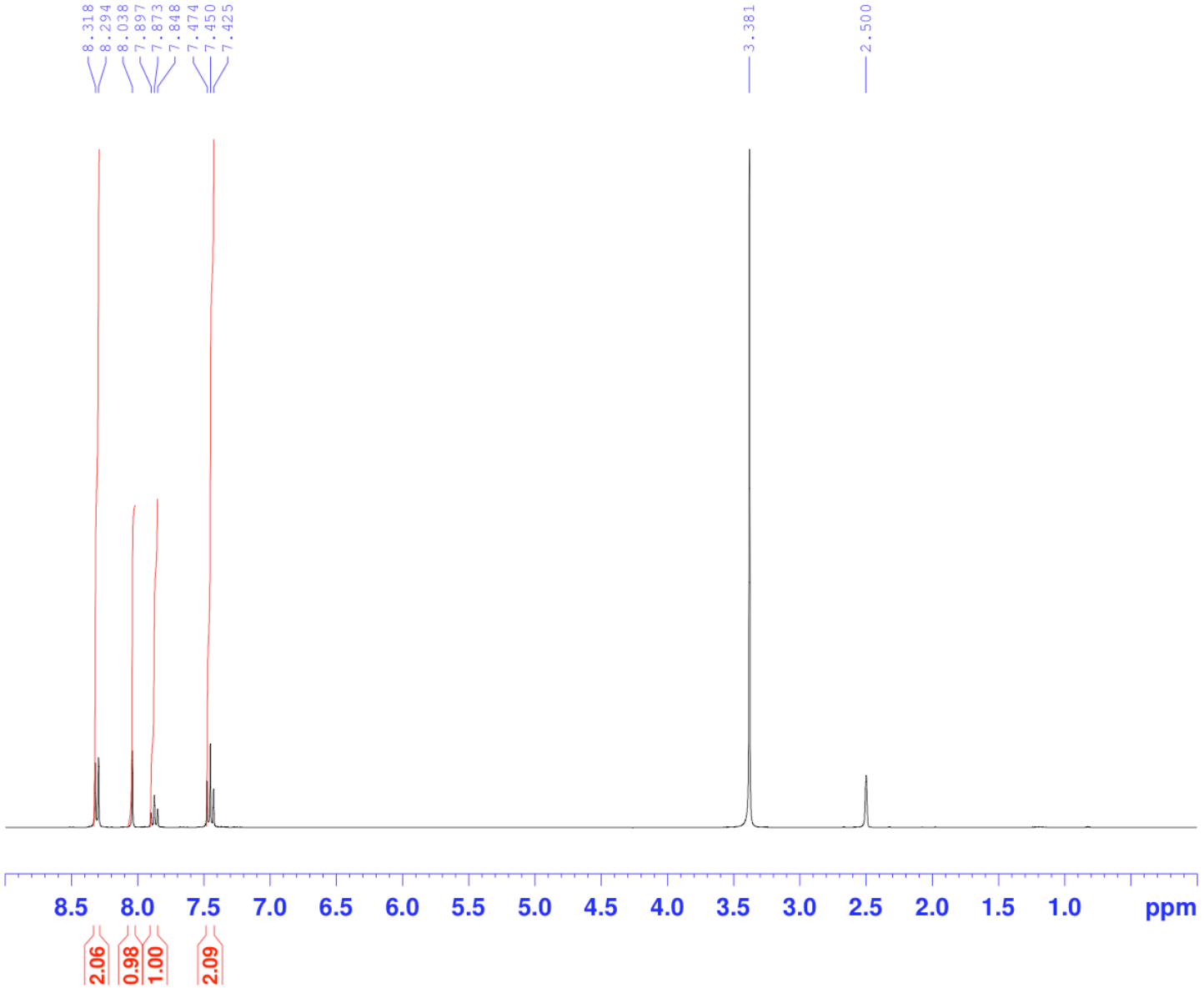
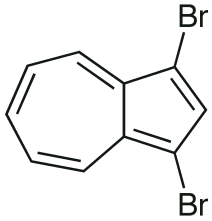
(400 MHz, DMSO-d_6)





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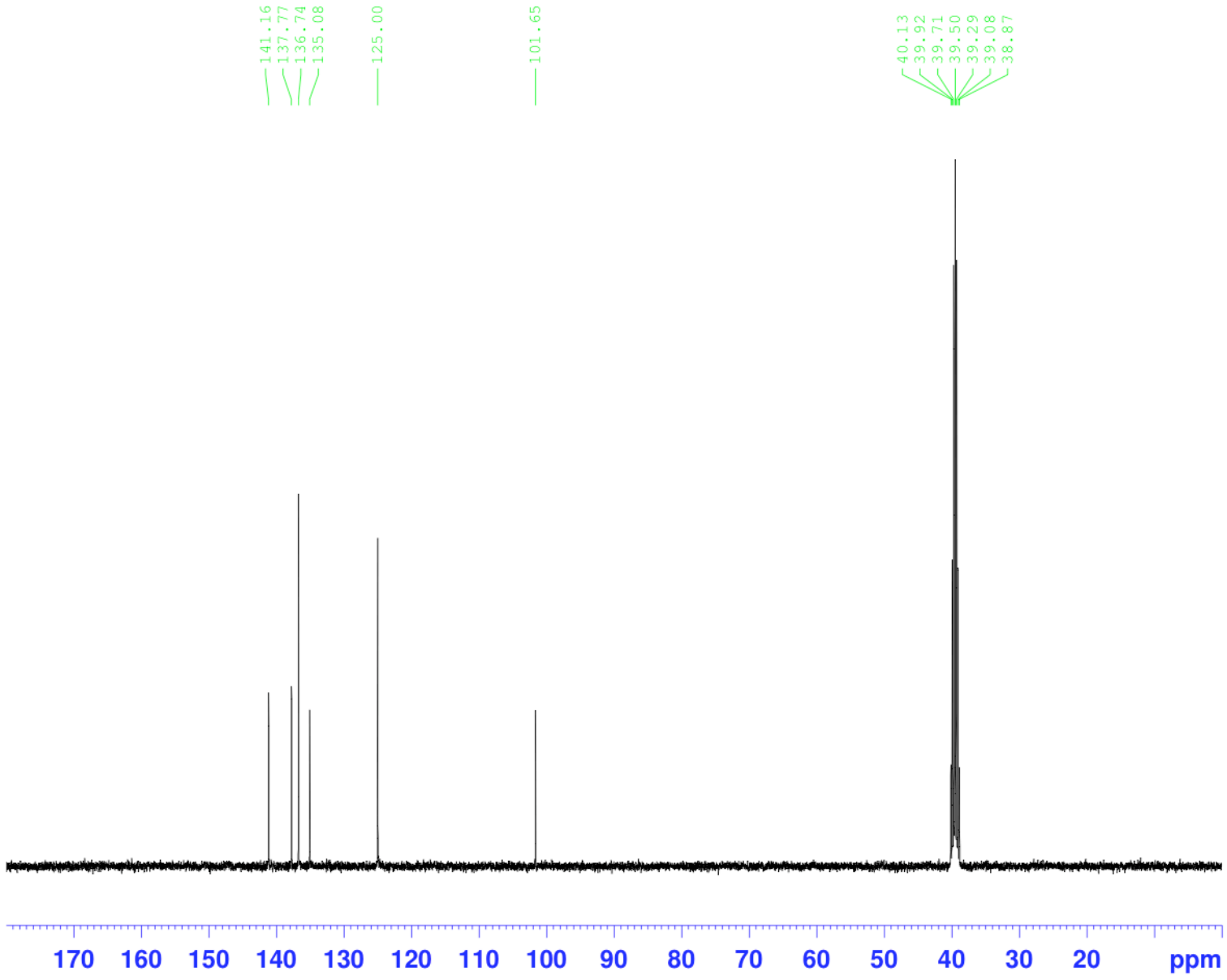
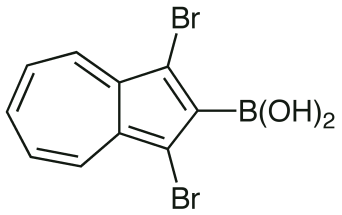
(100 MHz, DMSO-d_6)





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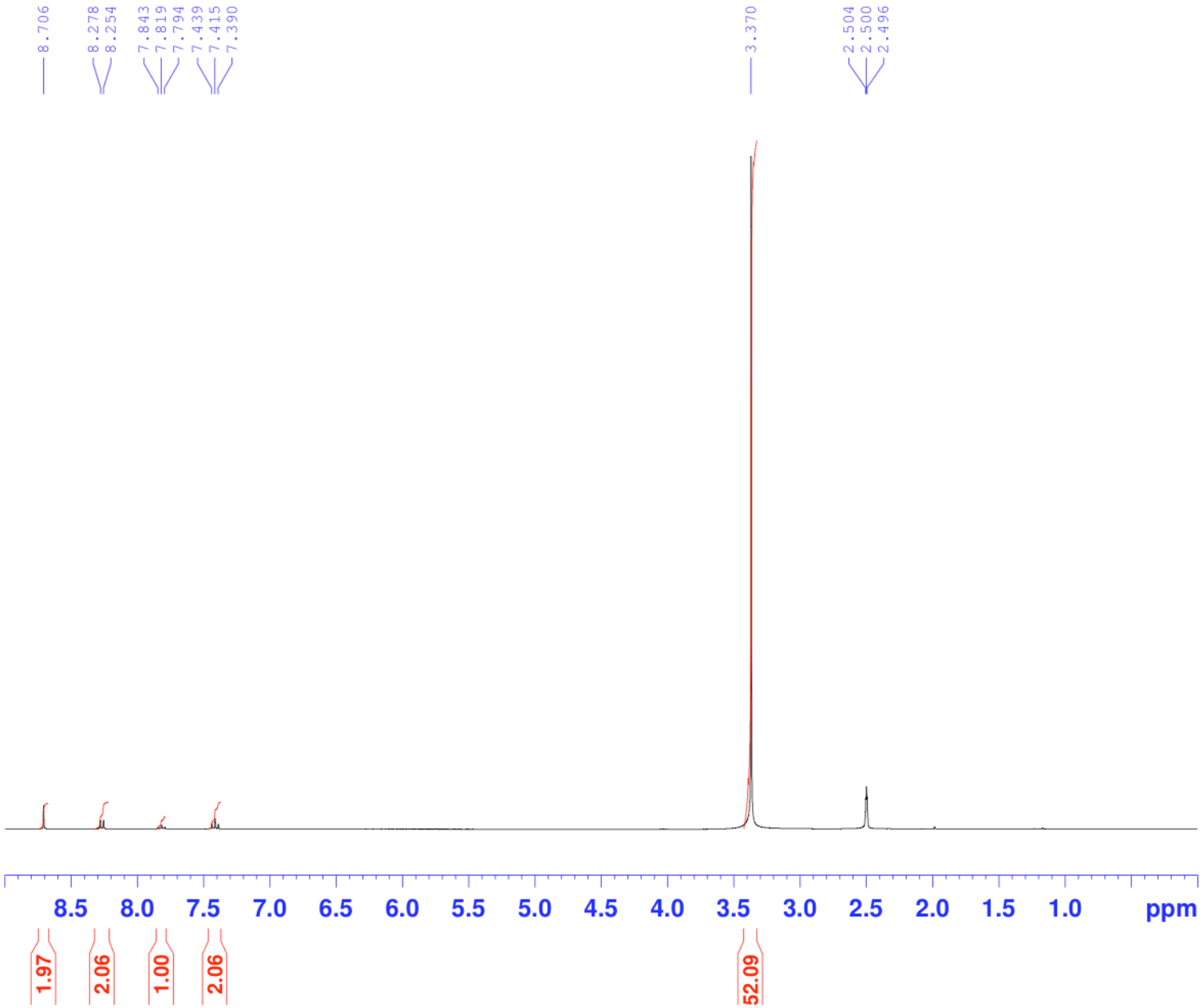
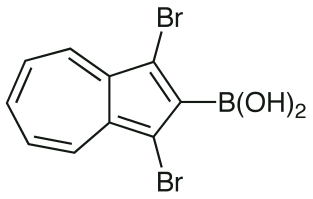
(400 MHz, DMSO-d_6)





6

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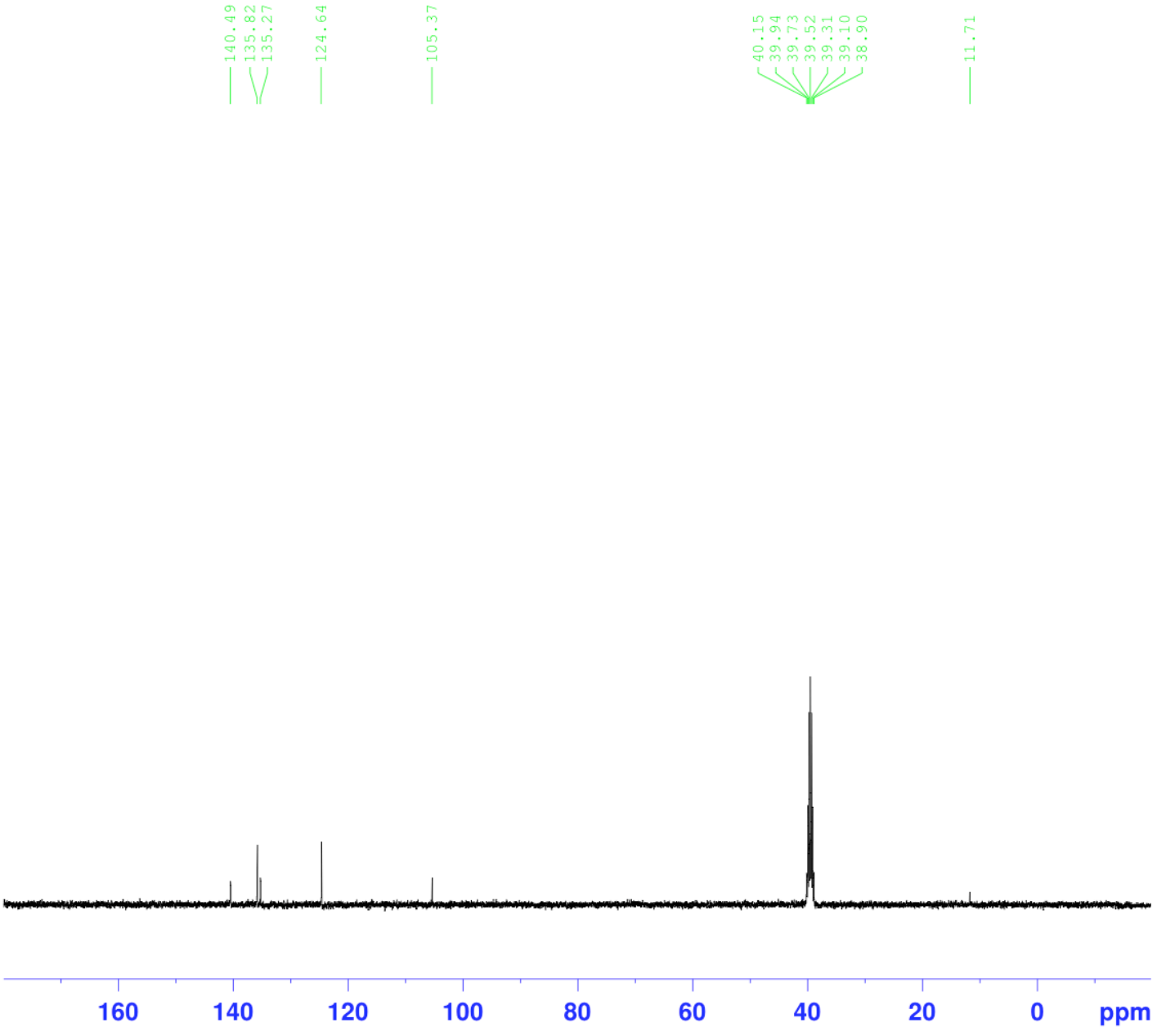
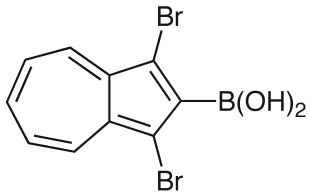
(100 MHz, DMSO-d_6)

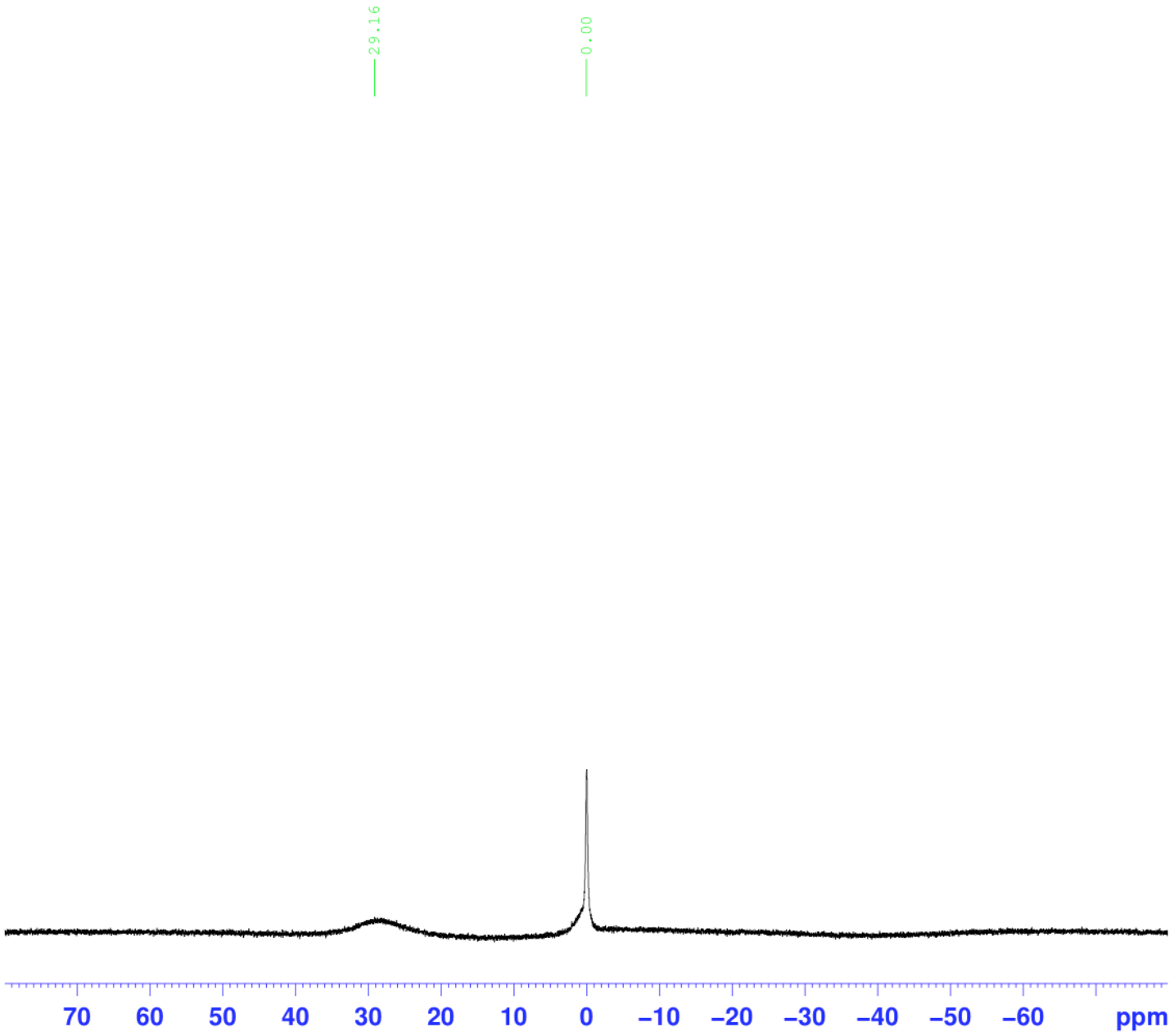


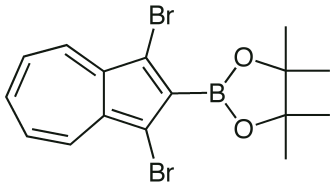


6

^{11}B NMR

(128 MHz, DMSO-d_6)

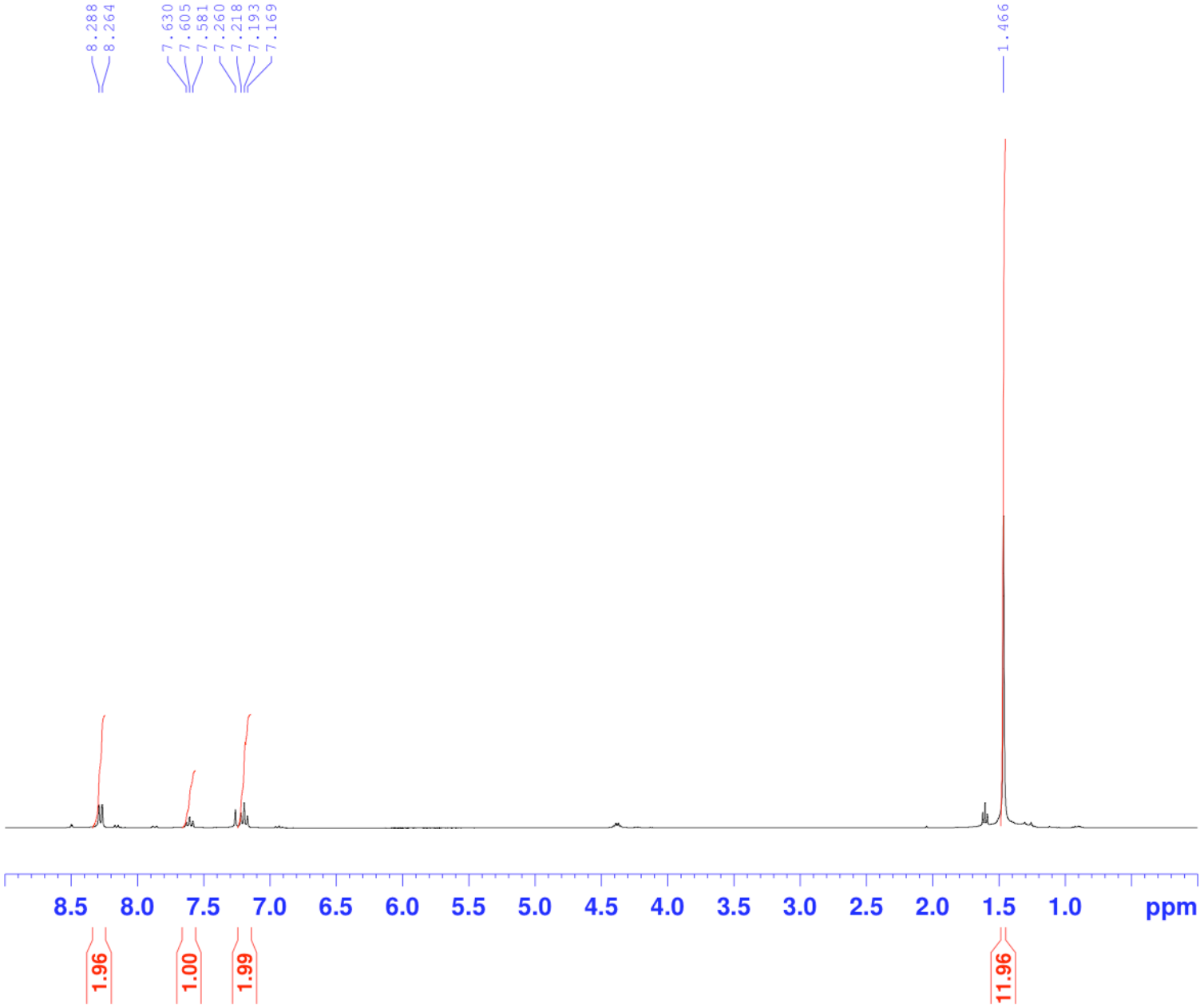


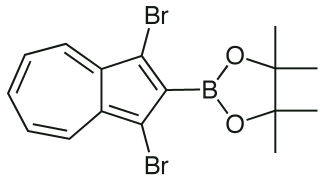


7a

^{1}H NMR

(400 MHz, $CDCl_3$)

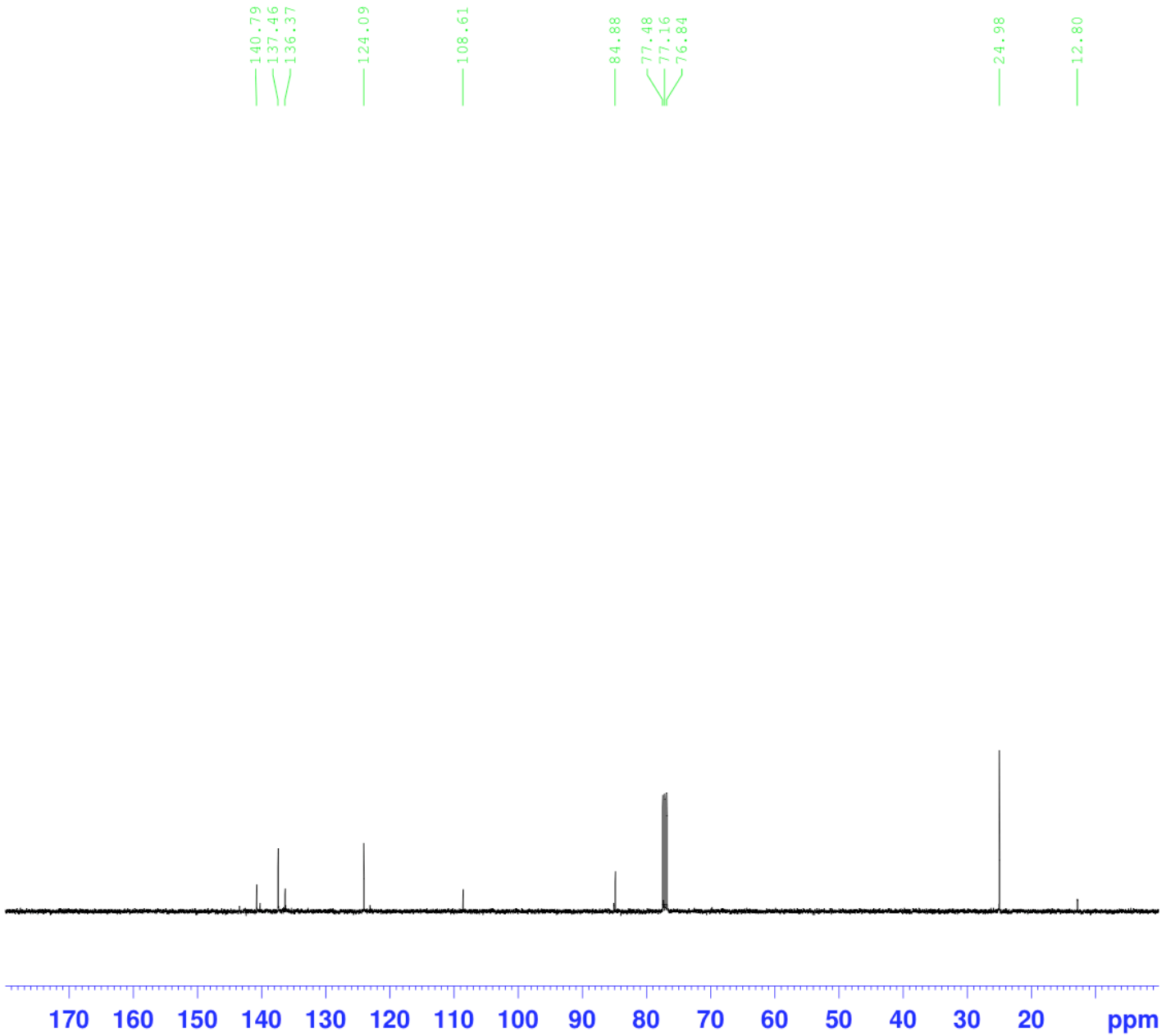


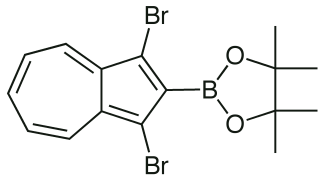


7a

^{13}C NMR

(100 MHz, $CDCl_3$)

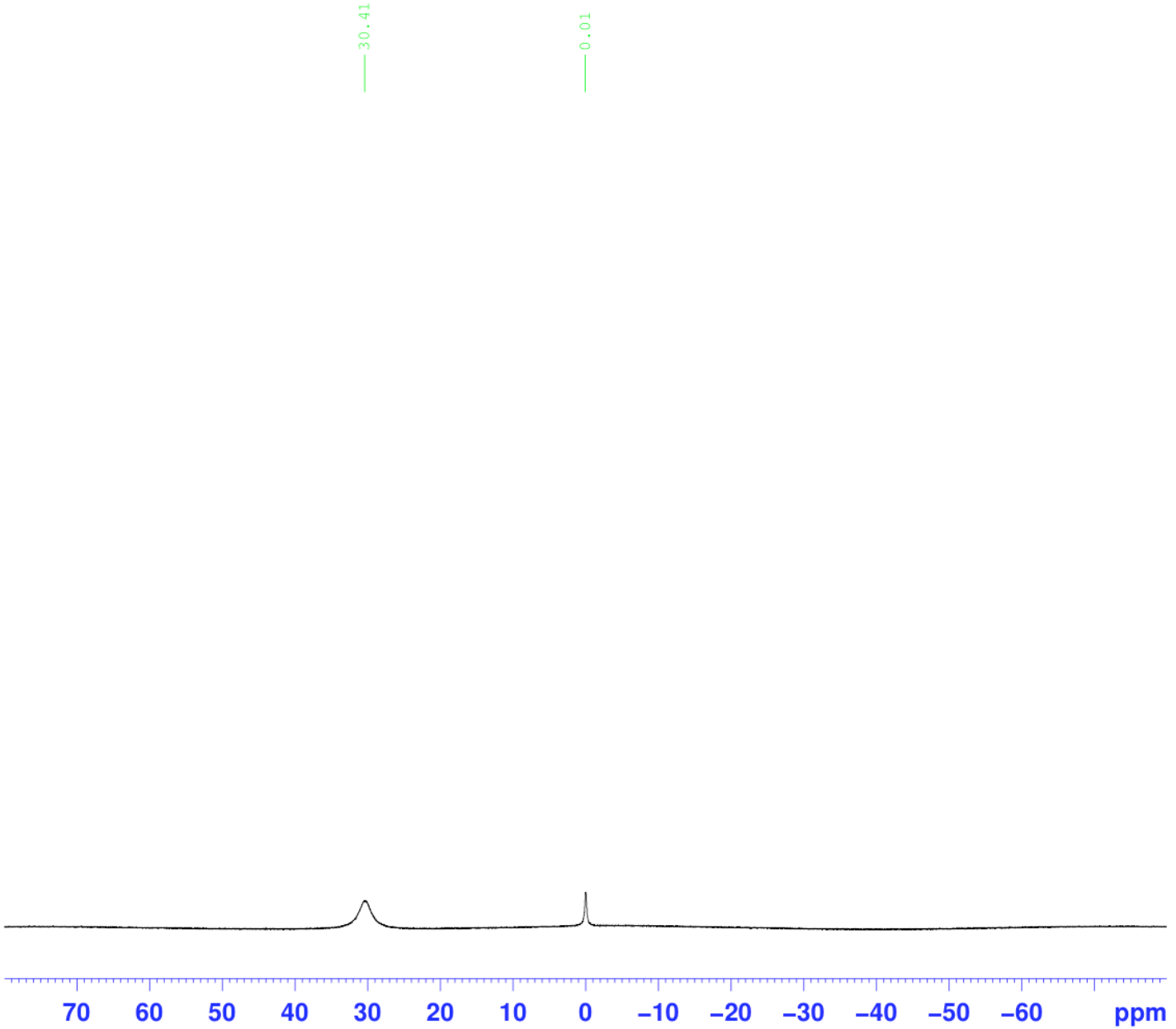


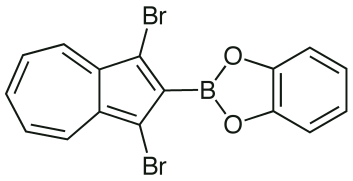


7a

^{11}B NMR

(128 MHz, $CDCl_3$)

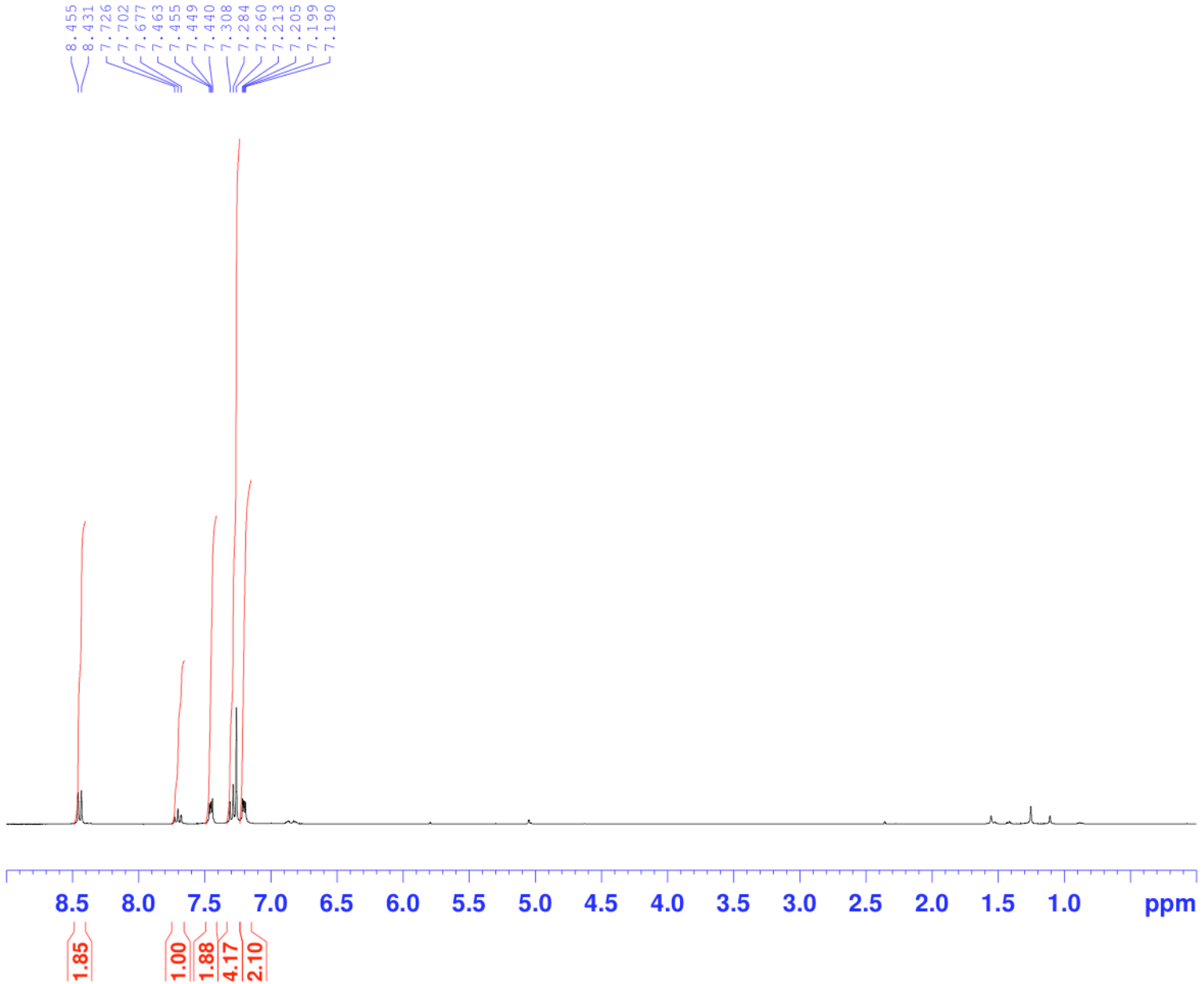


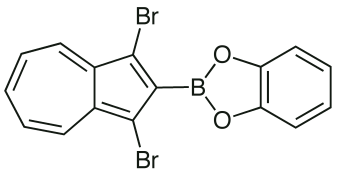


7b

^{1} H NMR

(400 MHz, $CDCl_3$)

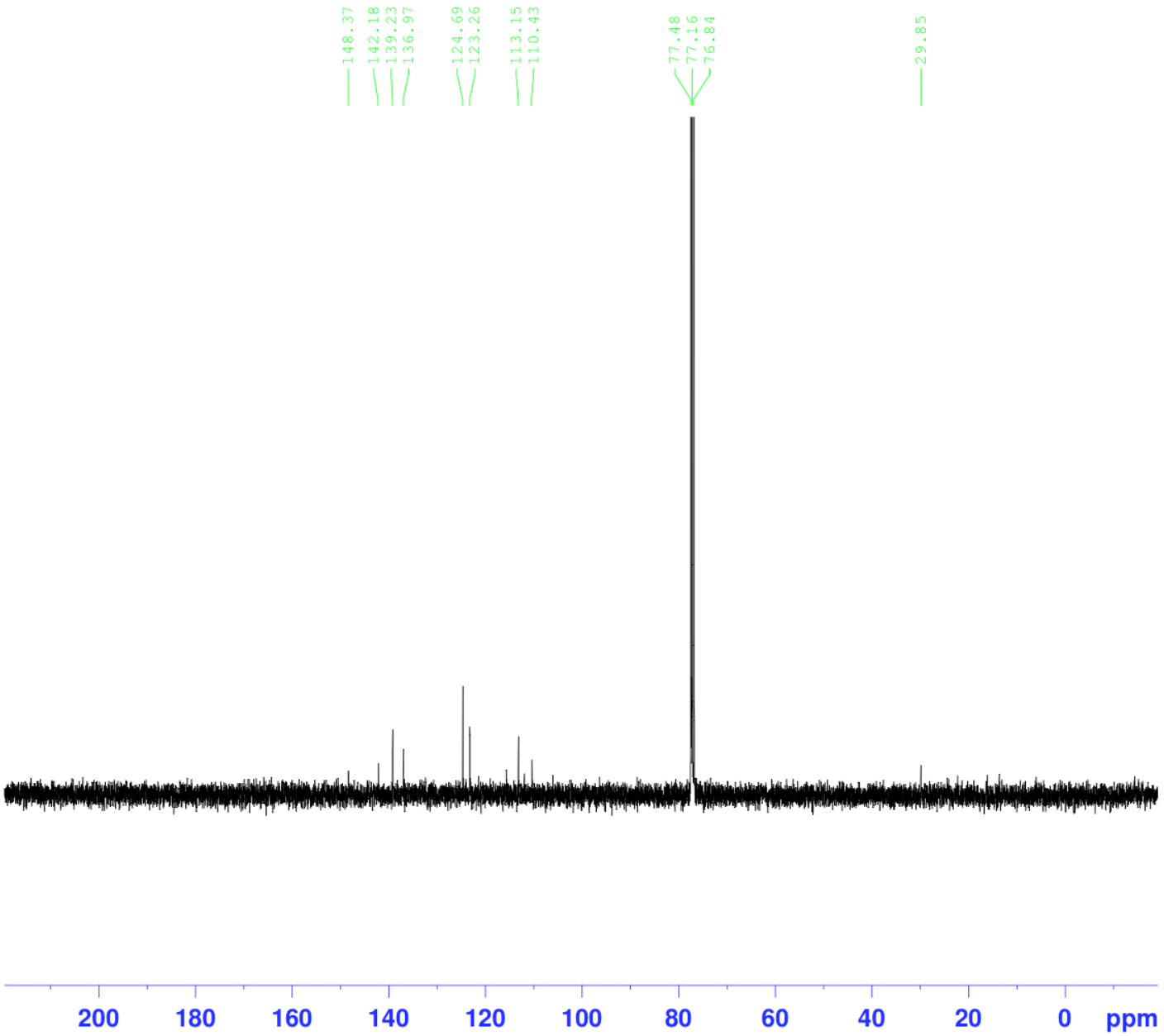


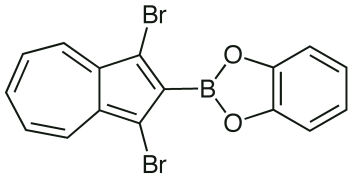


7b

^{13}C NMR

(100 MHz, $CDCl_3$)

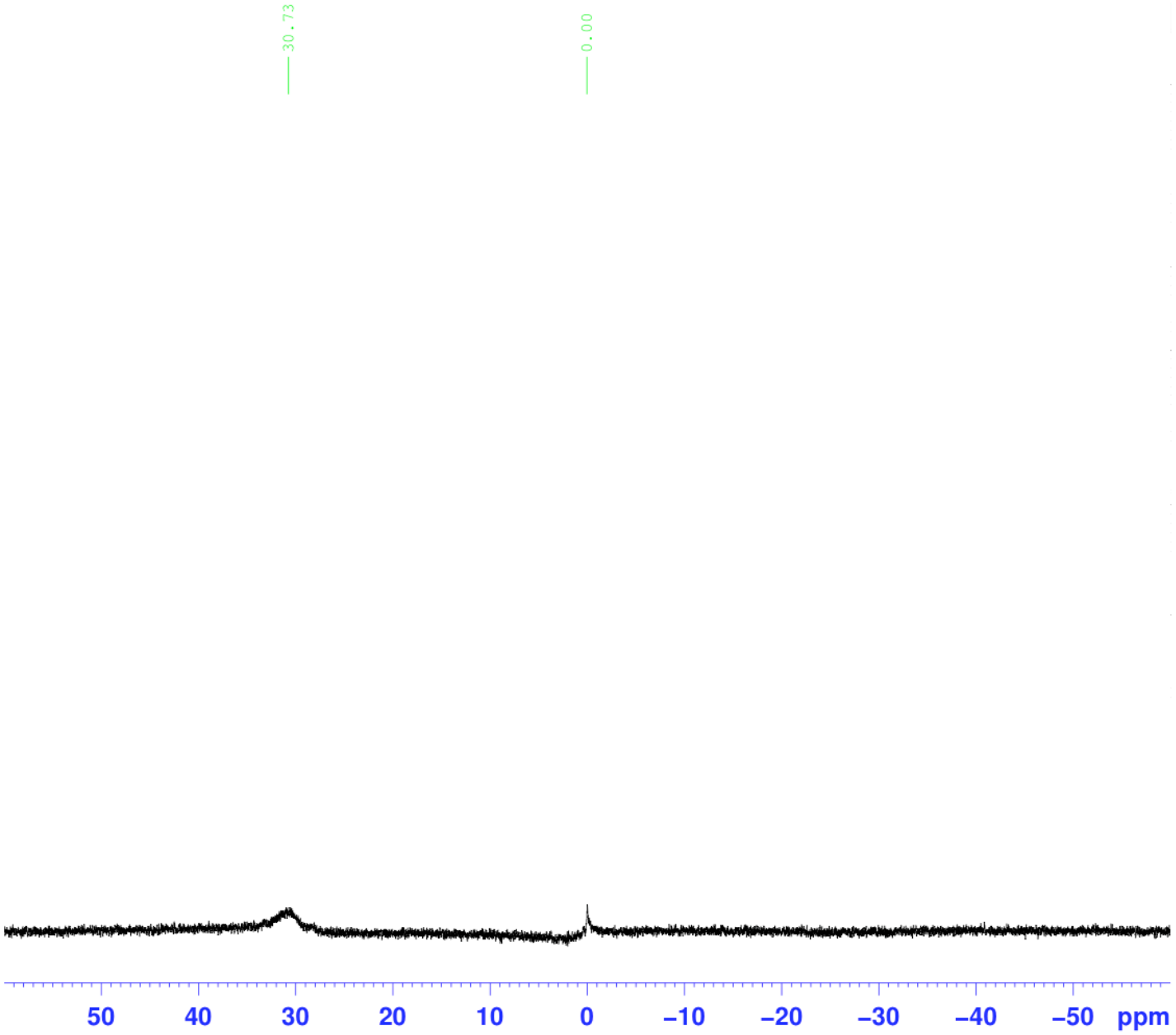


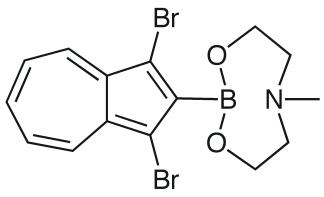


7b

^{11}B NMR

(128 MHz, $CDCl_3$)

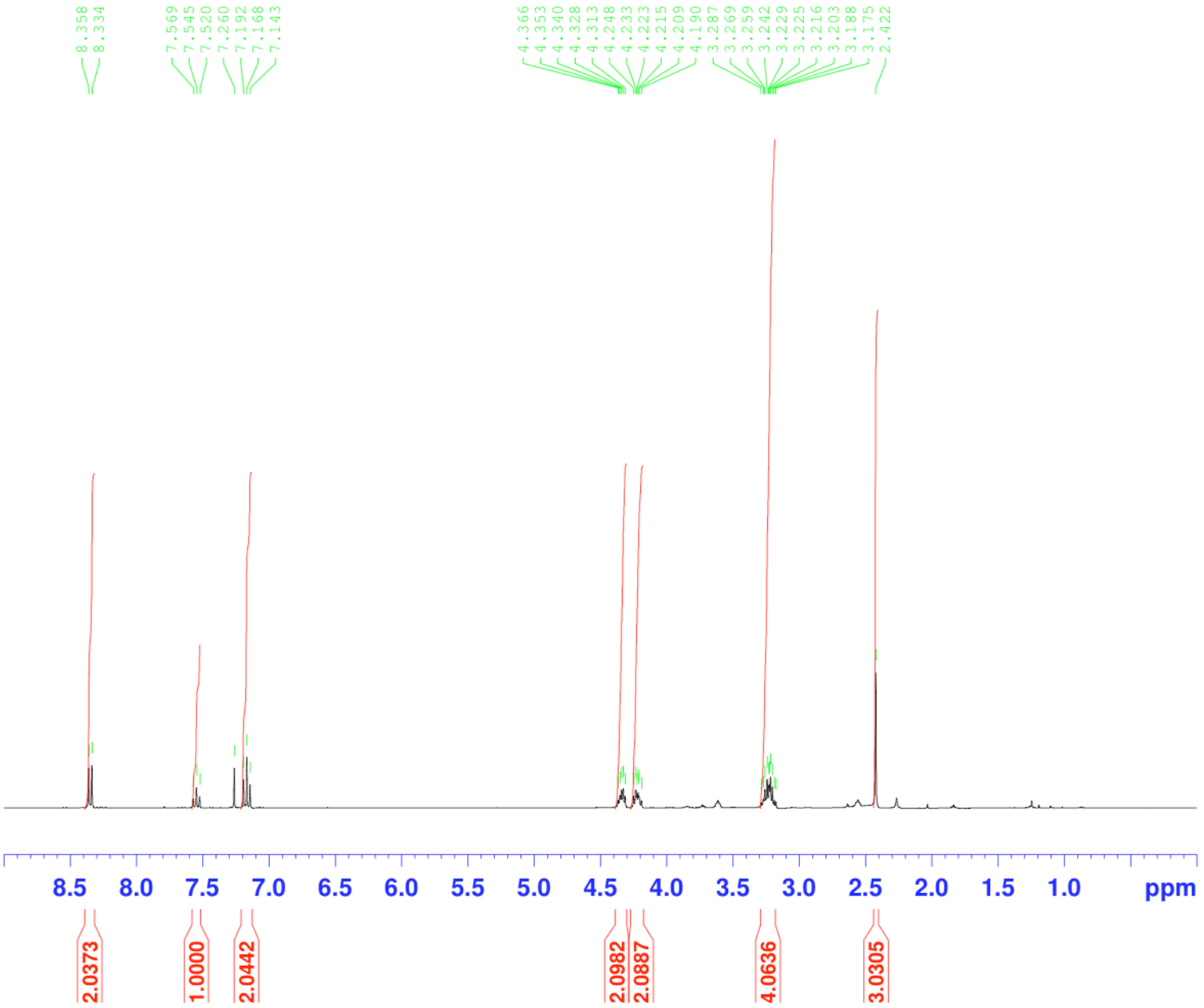


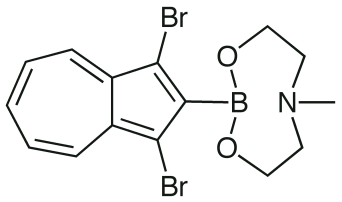


7c

^{1} H NMR

(400 MHz, $CDCl_3$)

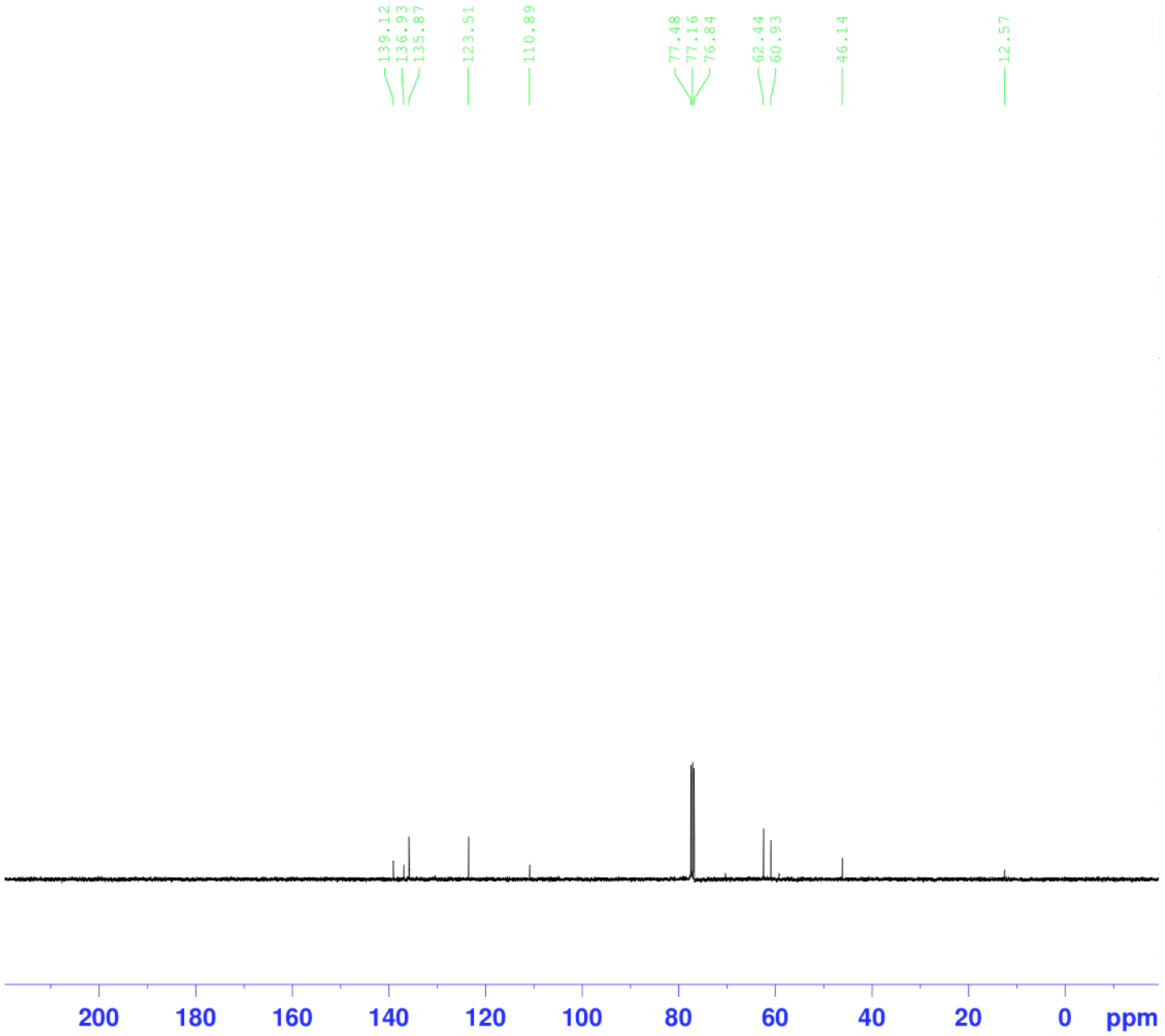


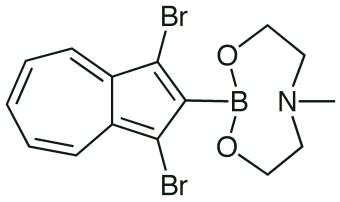


7c

^{13} C NMR

(100 MHz, $CDCl_3$)

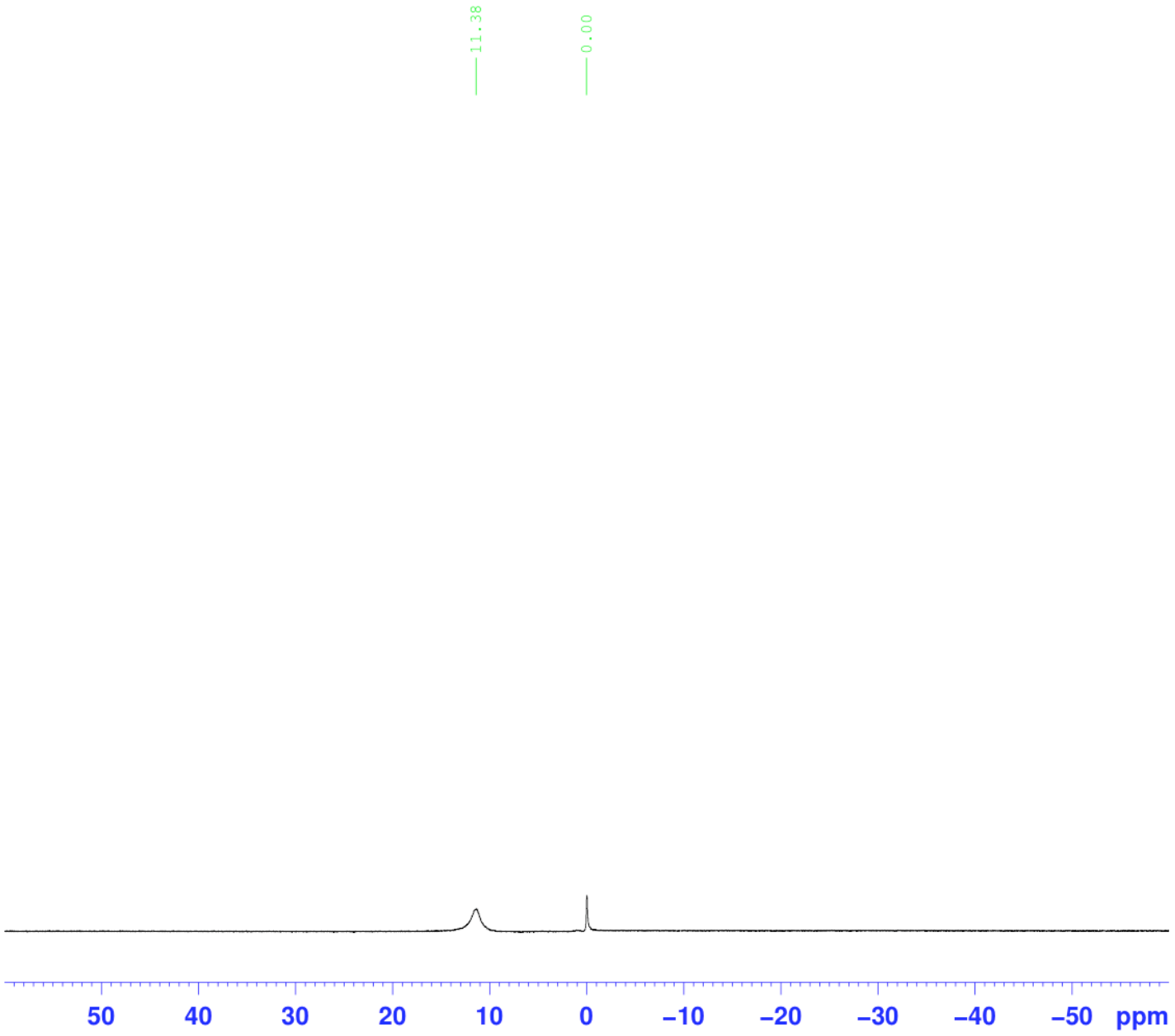


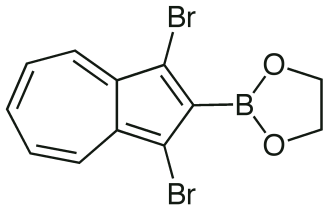


7c

^{11}B NMR

(128 MHz, $CDCl_3$)

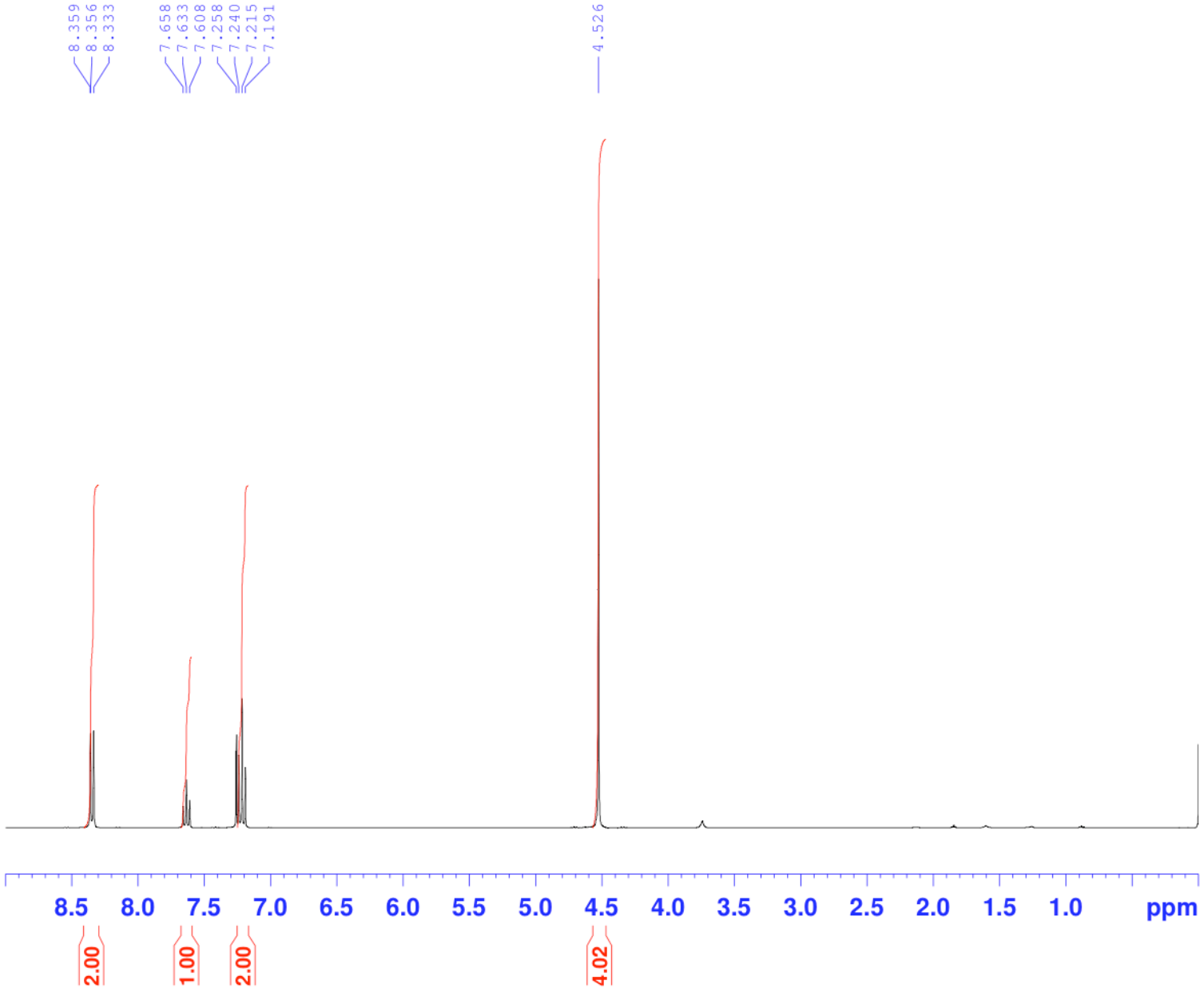


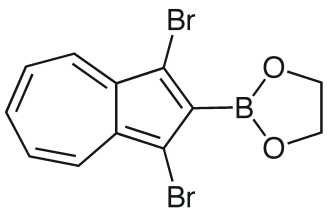


7d

^{1} H NMR

(400 MHz, $CDCl_3$)





7d

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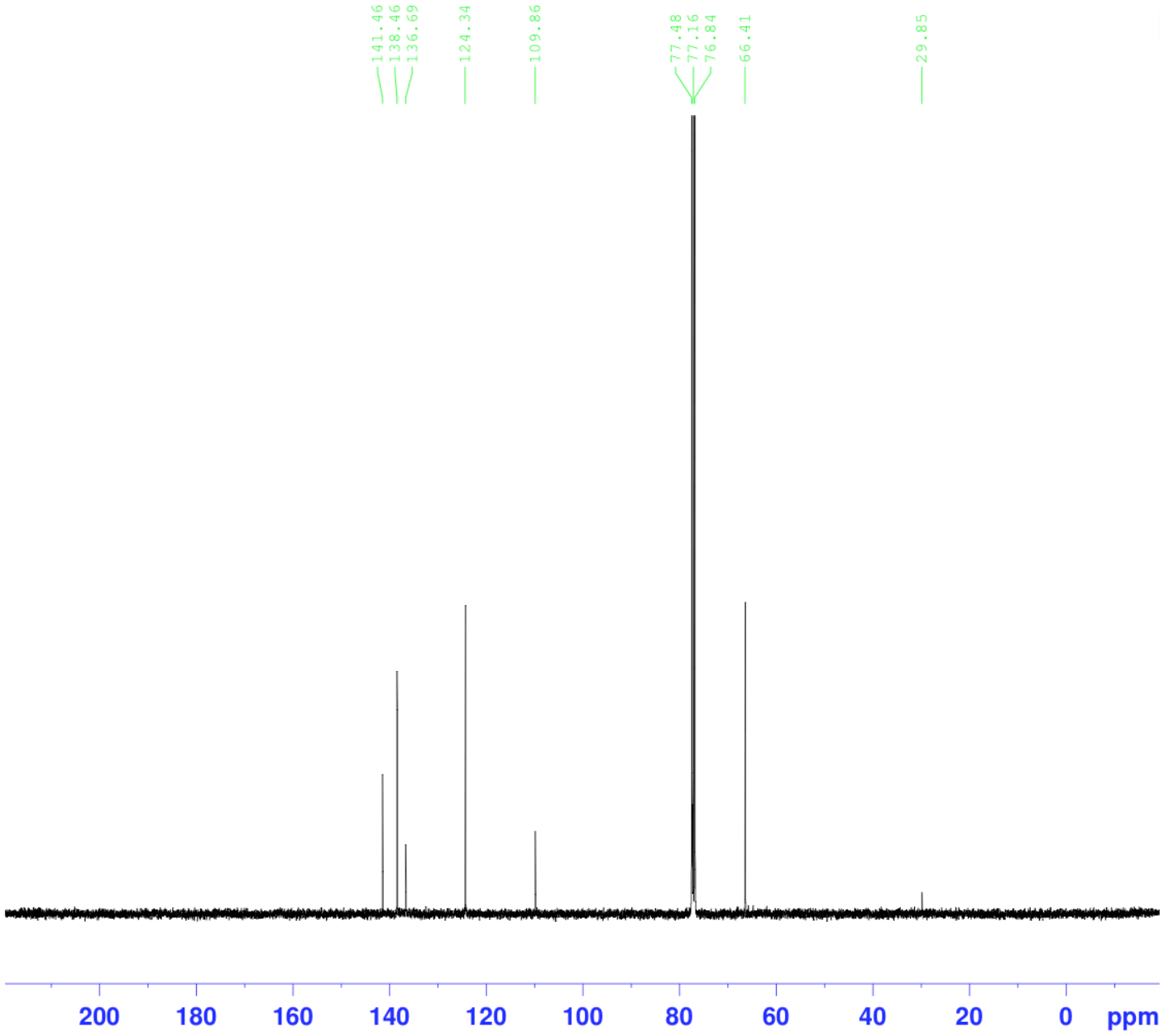
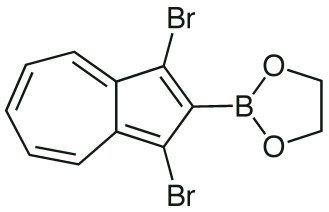
(100 MHz, $CDCl_3$)





7d

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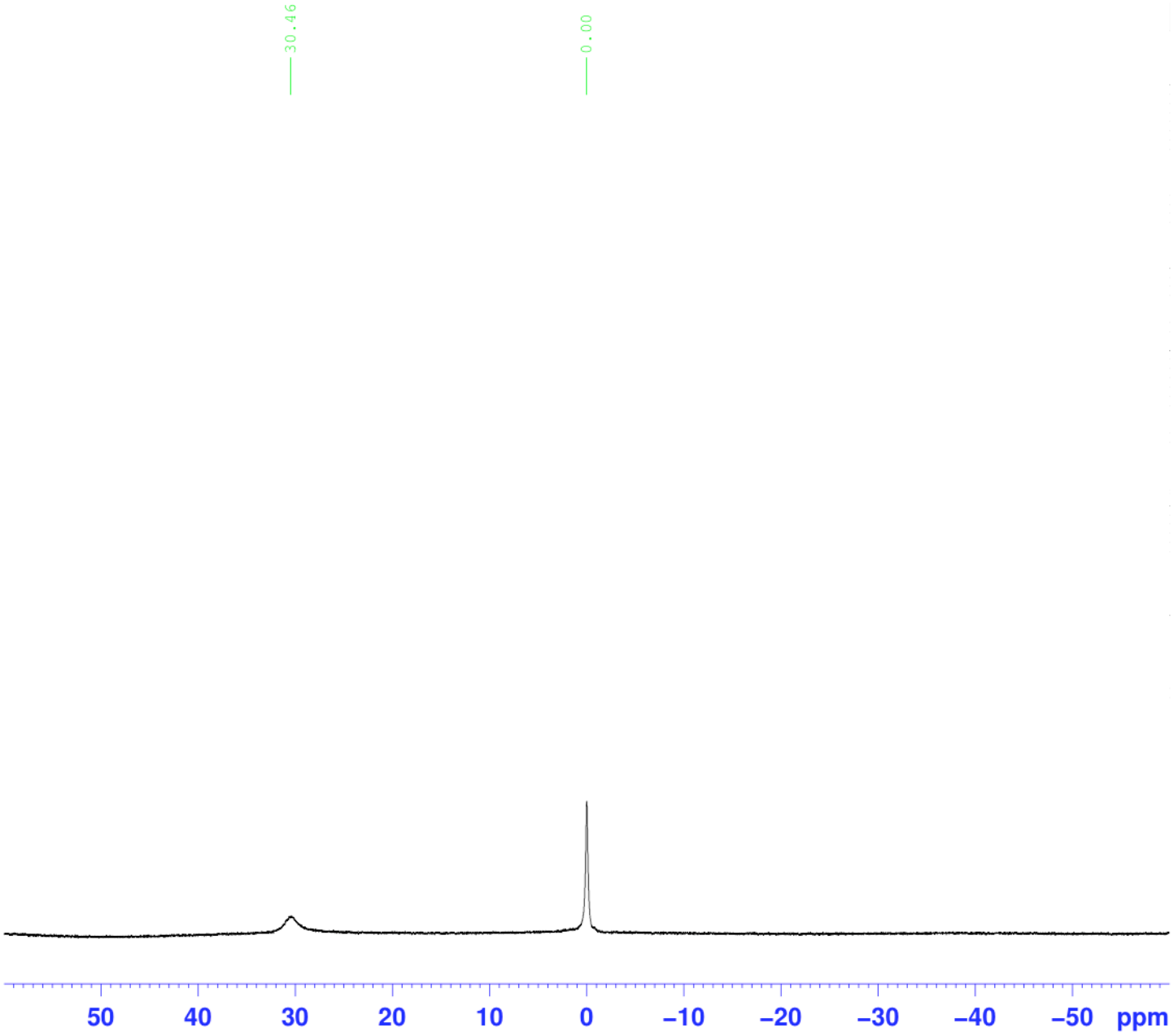
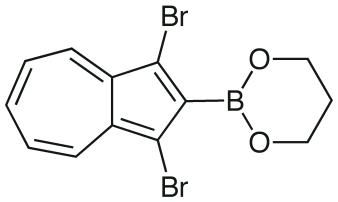
(128 MHz, $CDCl_3$)





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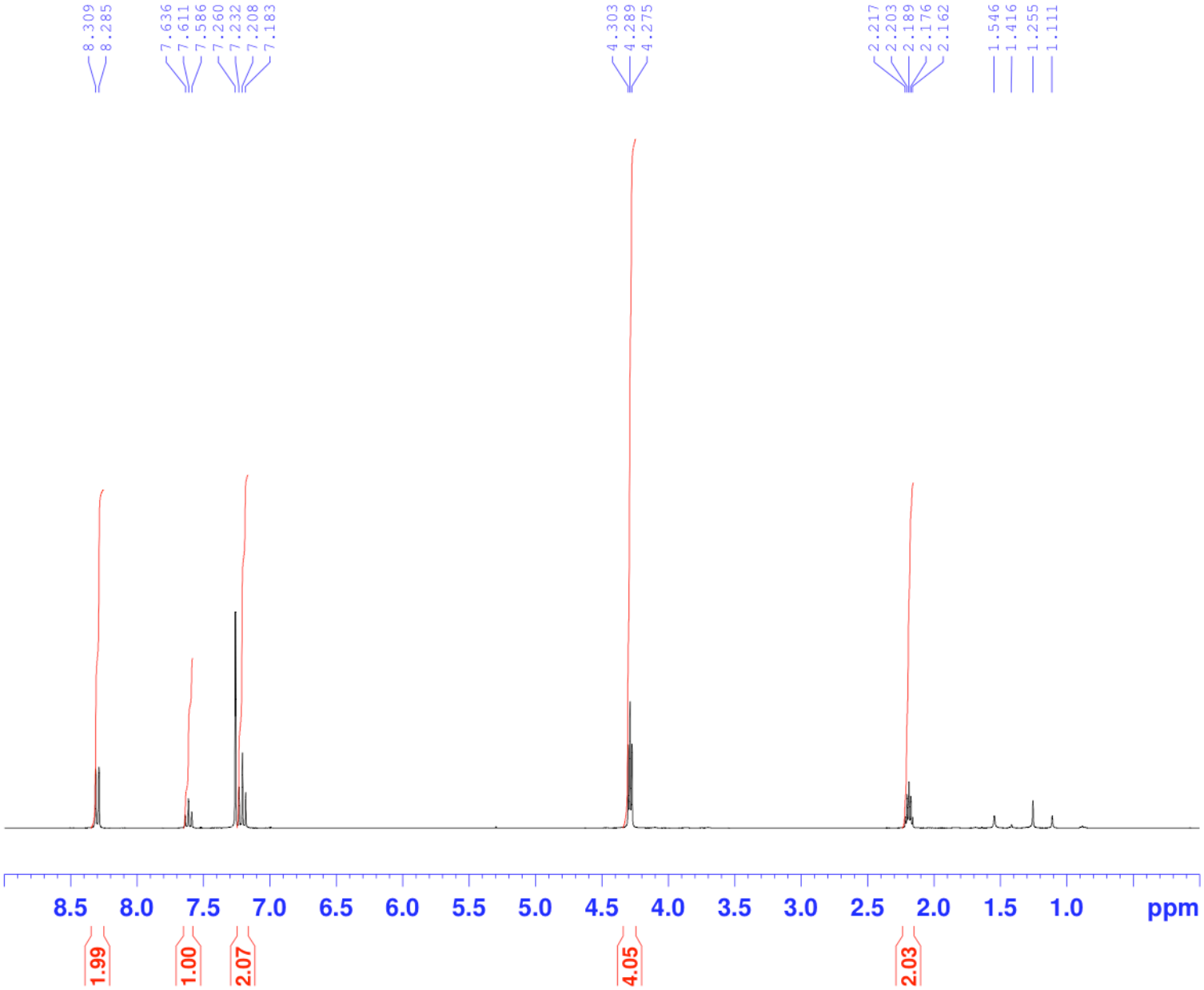
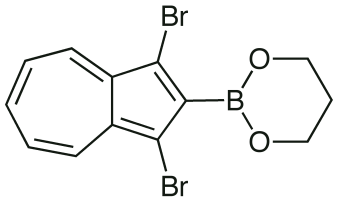
(400 MHz, $CDCl_3$)

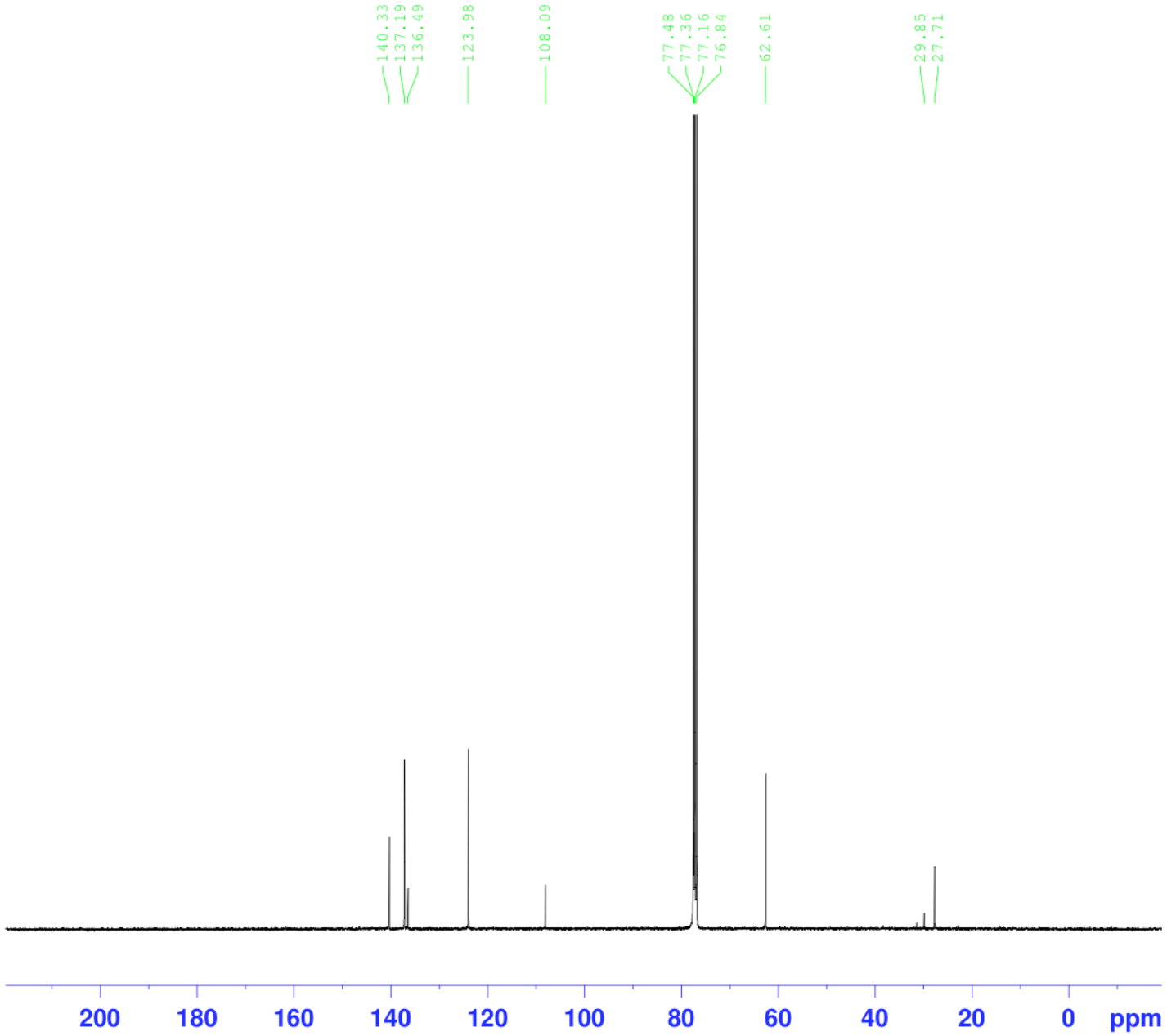


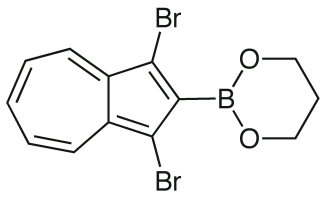


7e

^{13} C NMR

(100 MHz, $CDCl_3$)

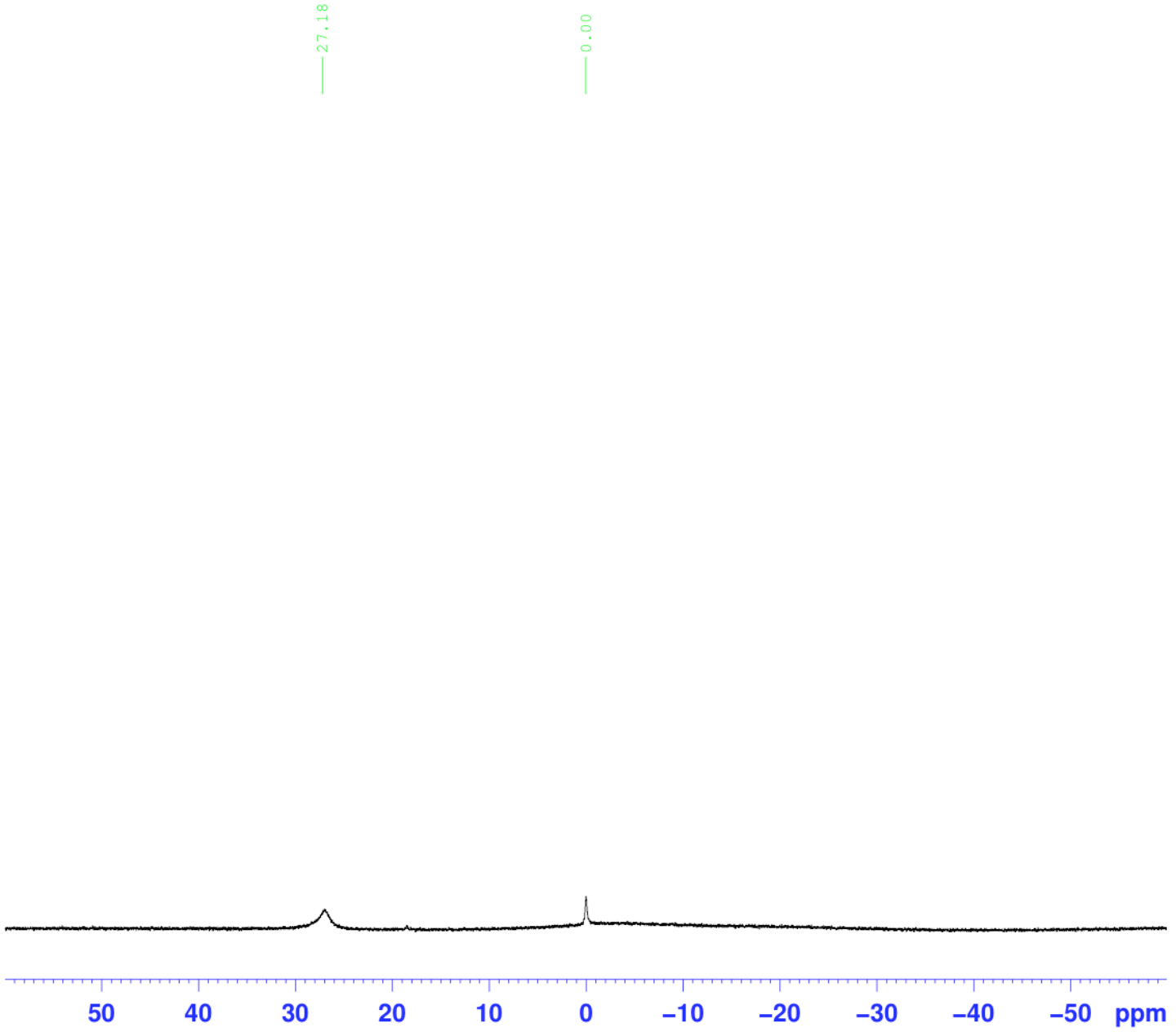


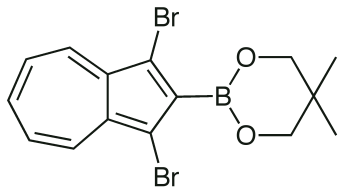


7e

^{11} B NMR

(128 MHz, $CDCl_3$)

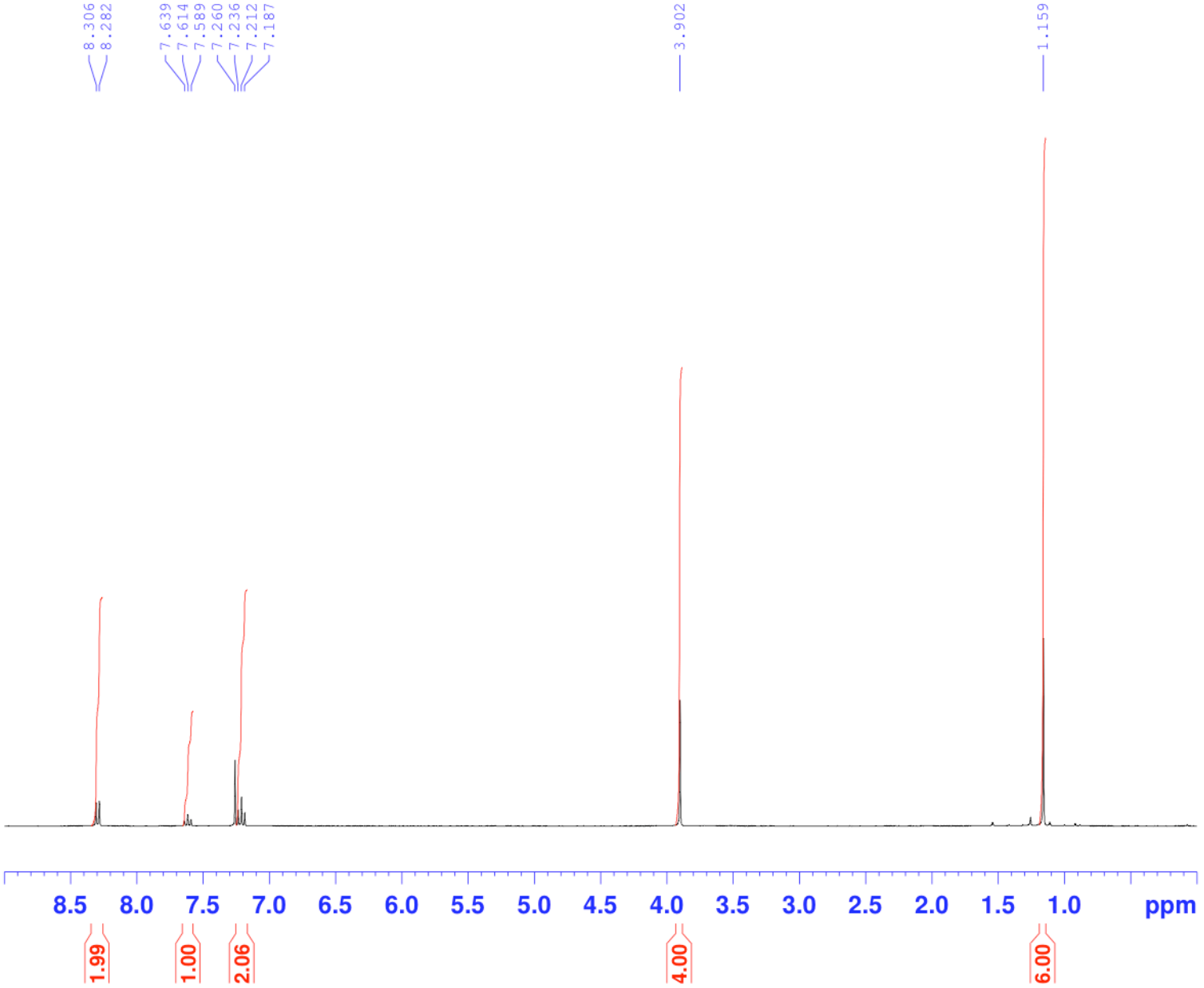


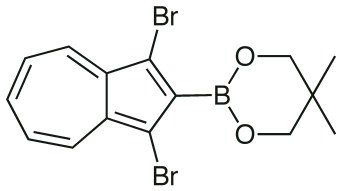


7f

^{1} H NMR

(400 MHz, $CDCl_3$)

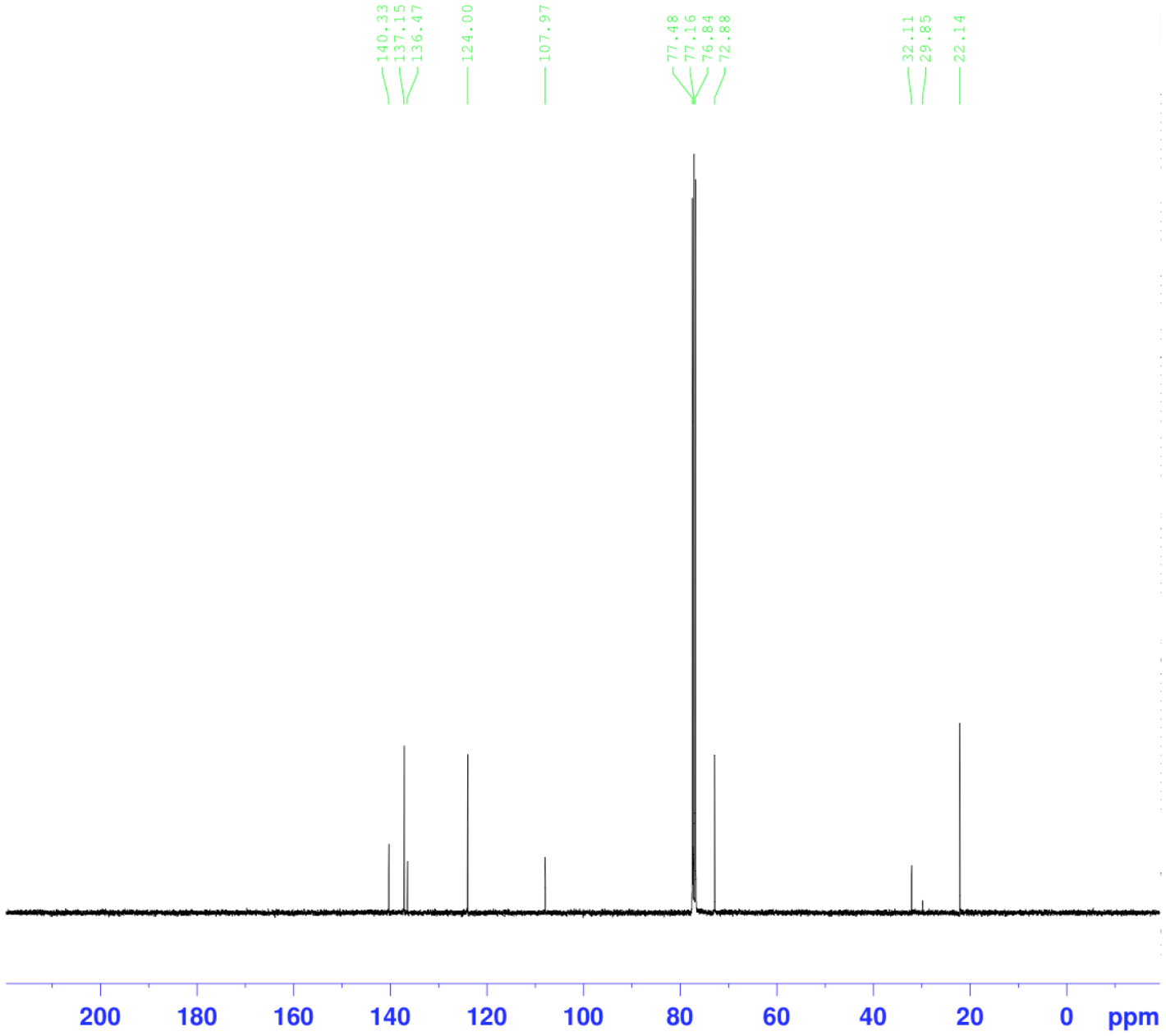


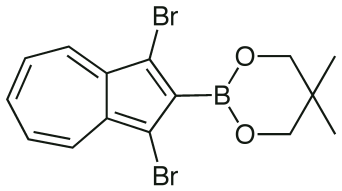


7f

^{13}C NMR

(100 MHz, $CDCl_3$)

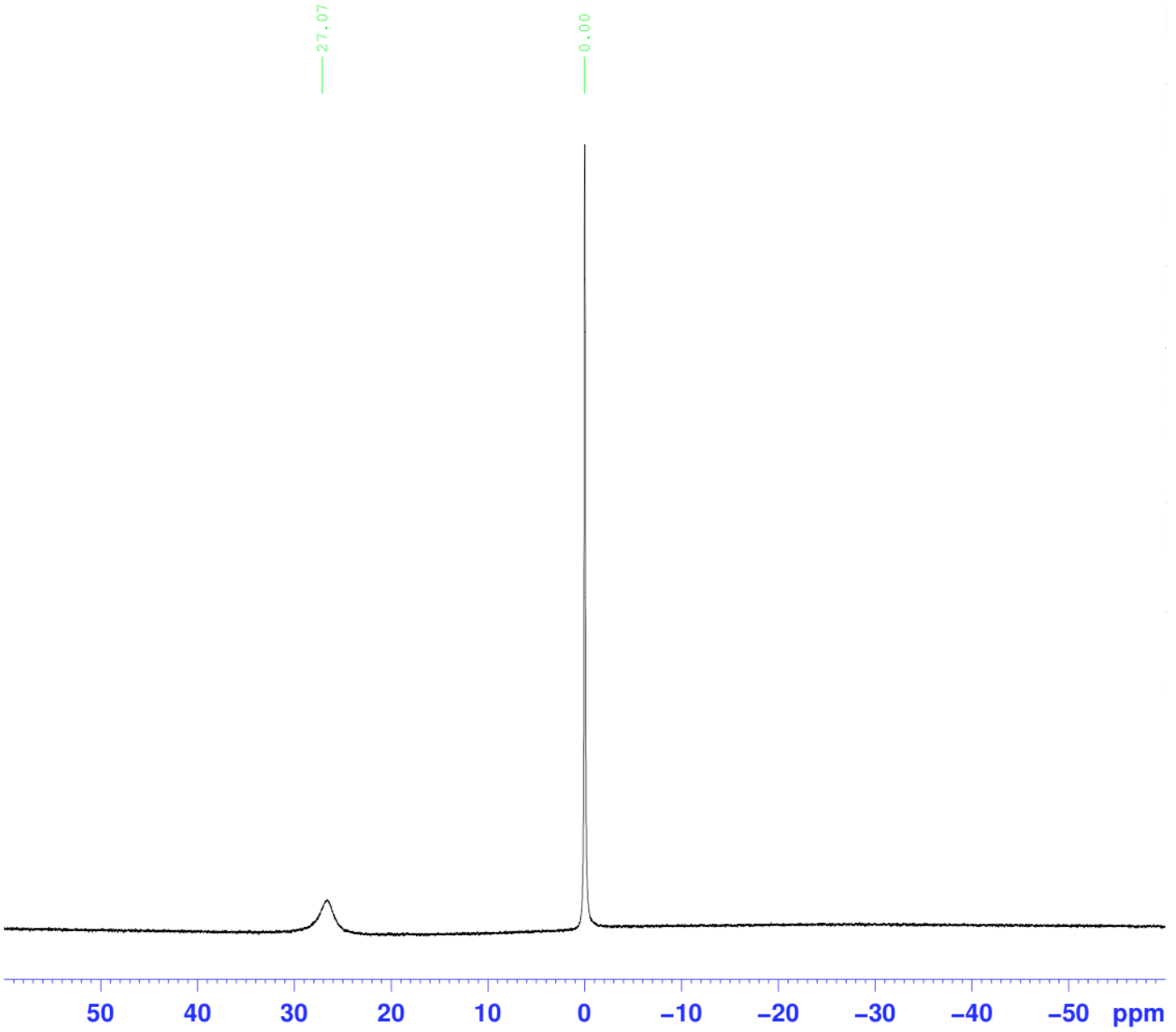


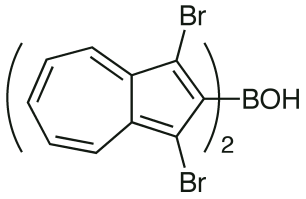


7f

^{11}B NMR

(128 MHz, $CDCl_3$)

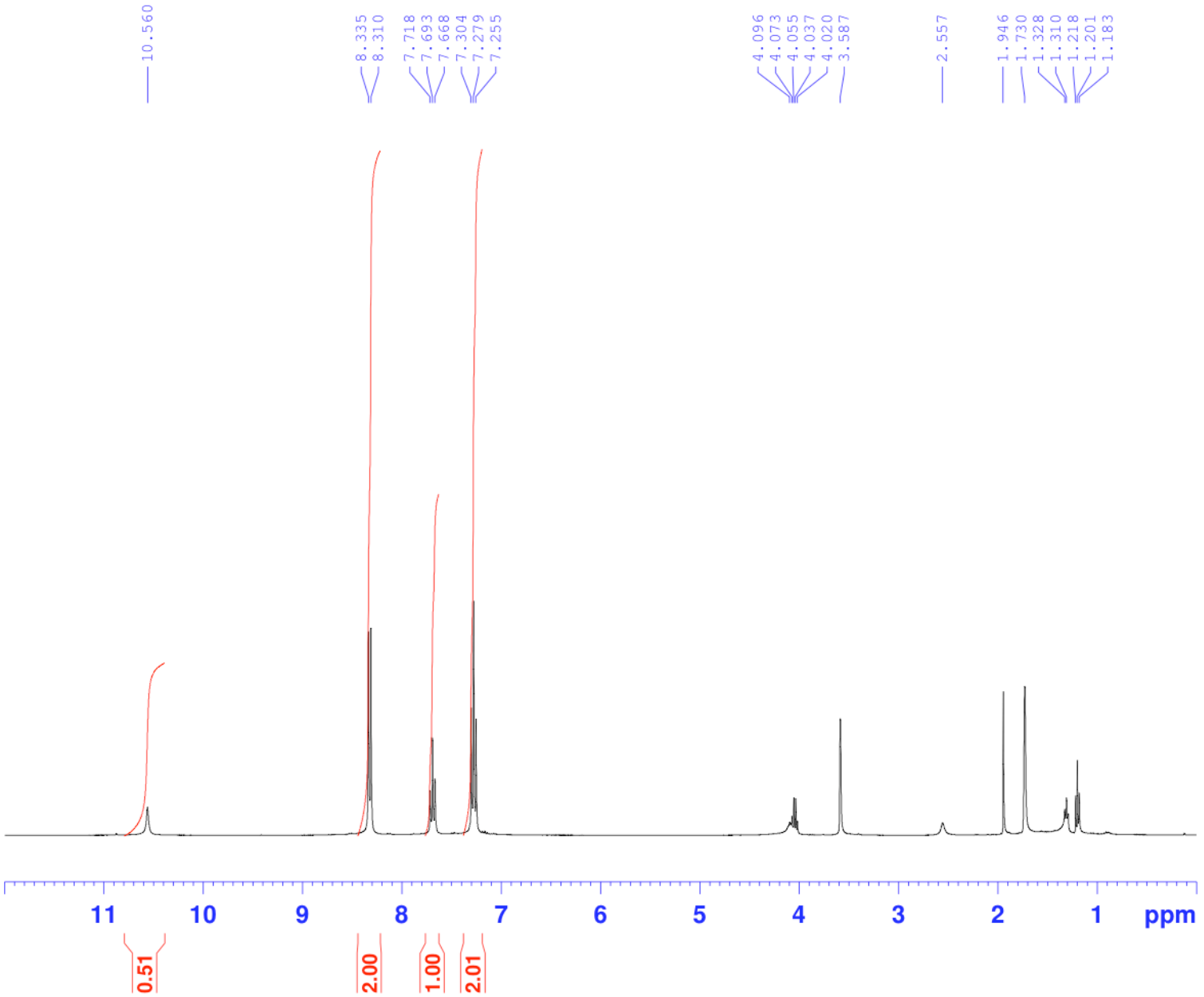




1

^{1}H NMR

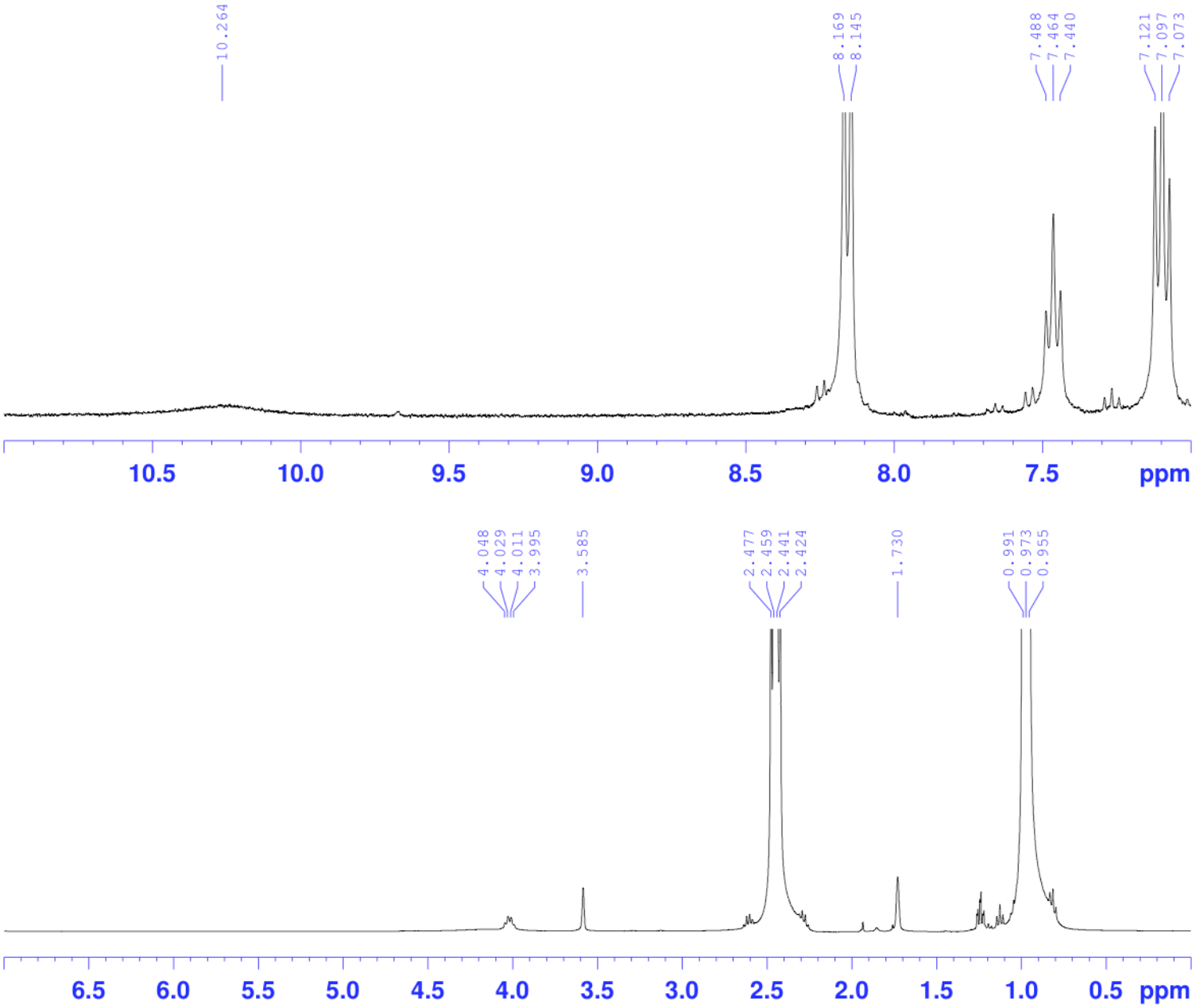
(400 MHz, THF-d_8)

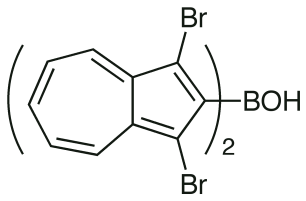


1 + Et_3N

^{1}H NMR

(400 MHz, THF-d_8)

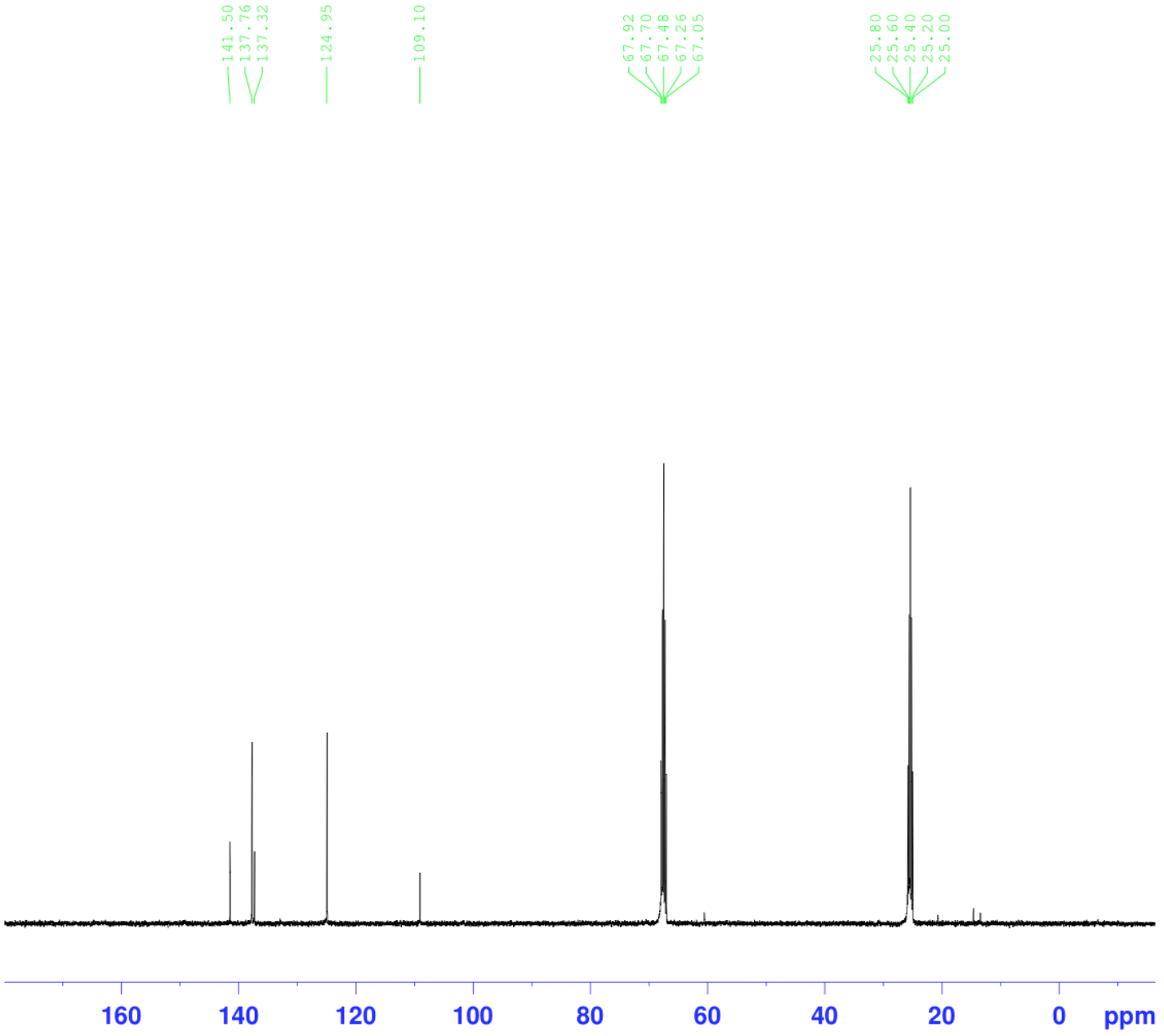




1

^{13}C NMR

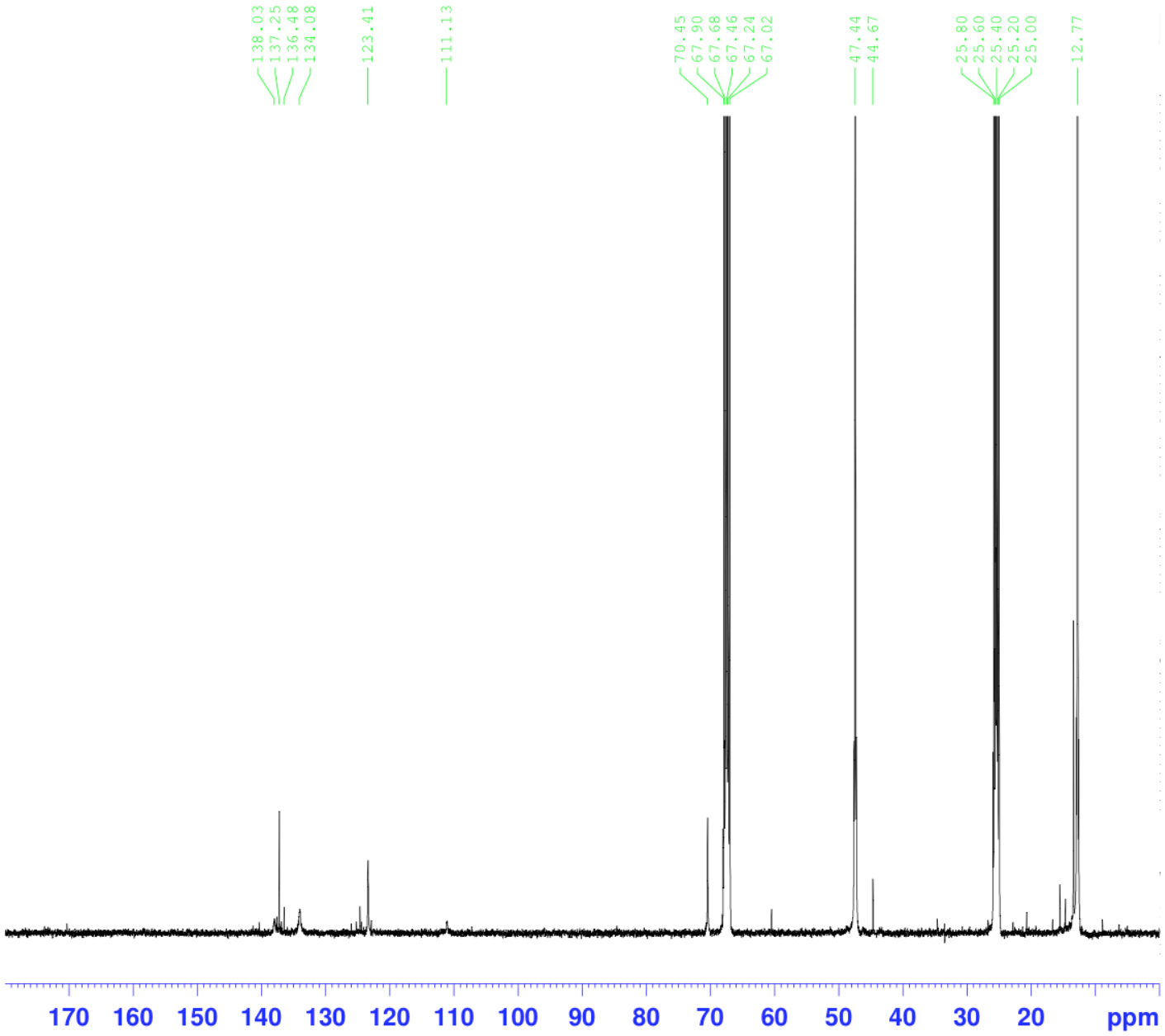
(100 MHz, THF-d_8)



1 + Et_3N

^{13}C NMR

(100 MHz, THF-d_8)

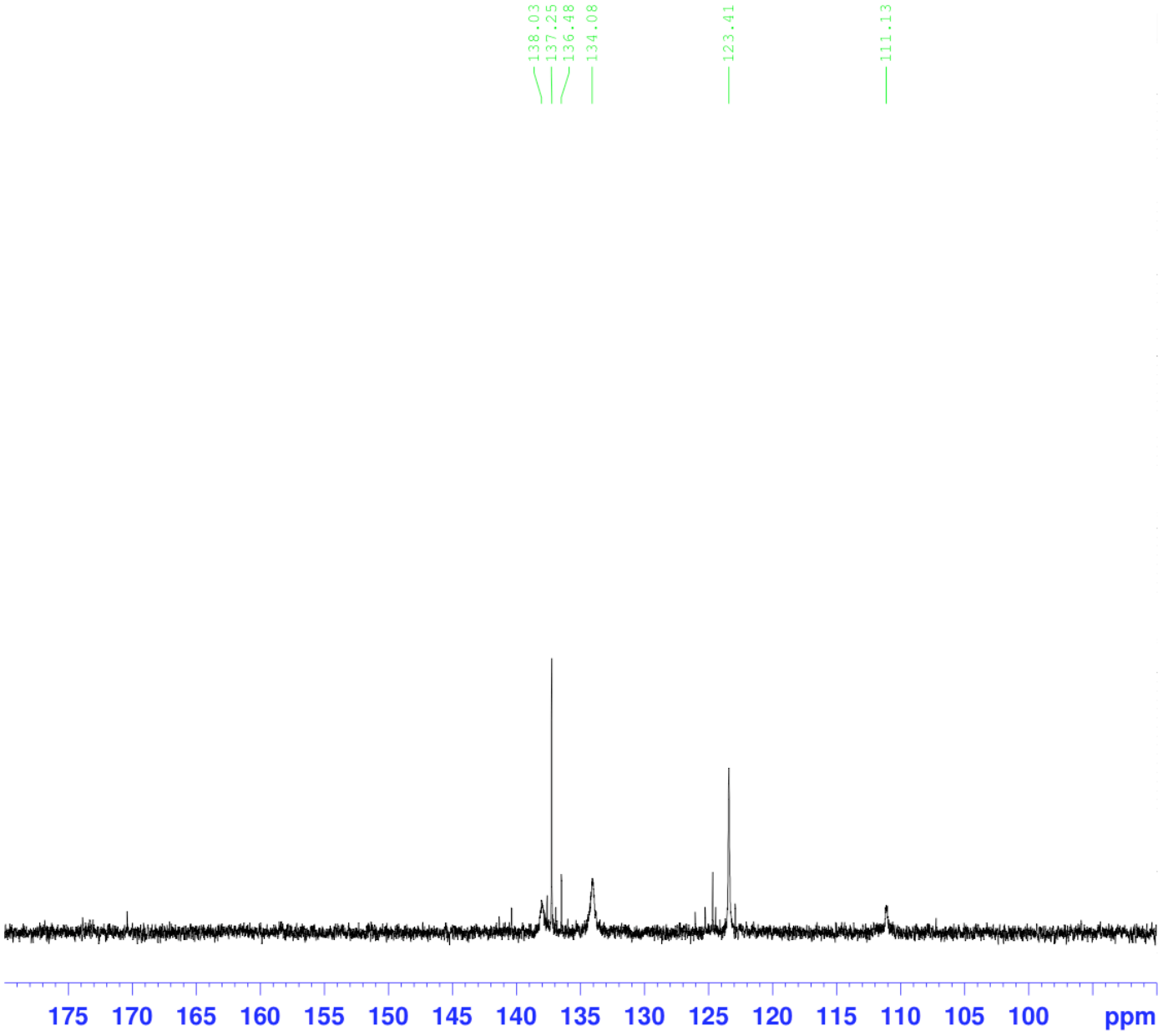


1 + Et_3N

^{13}C NMR

(100 MHz, THF-d_8)

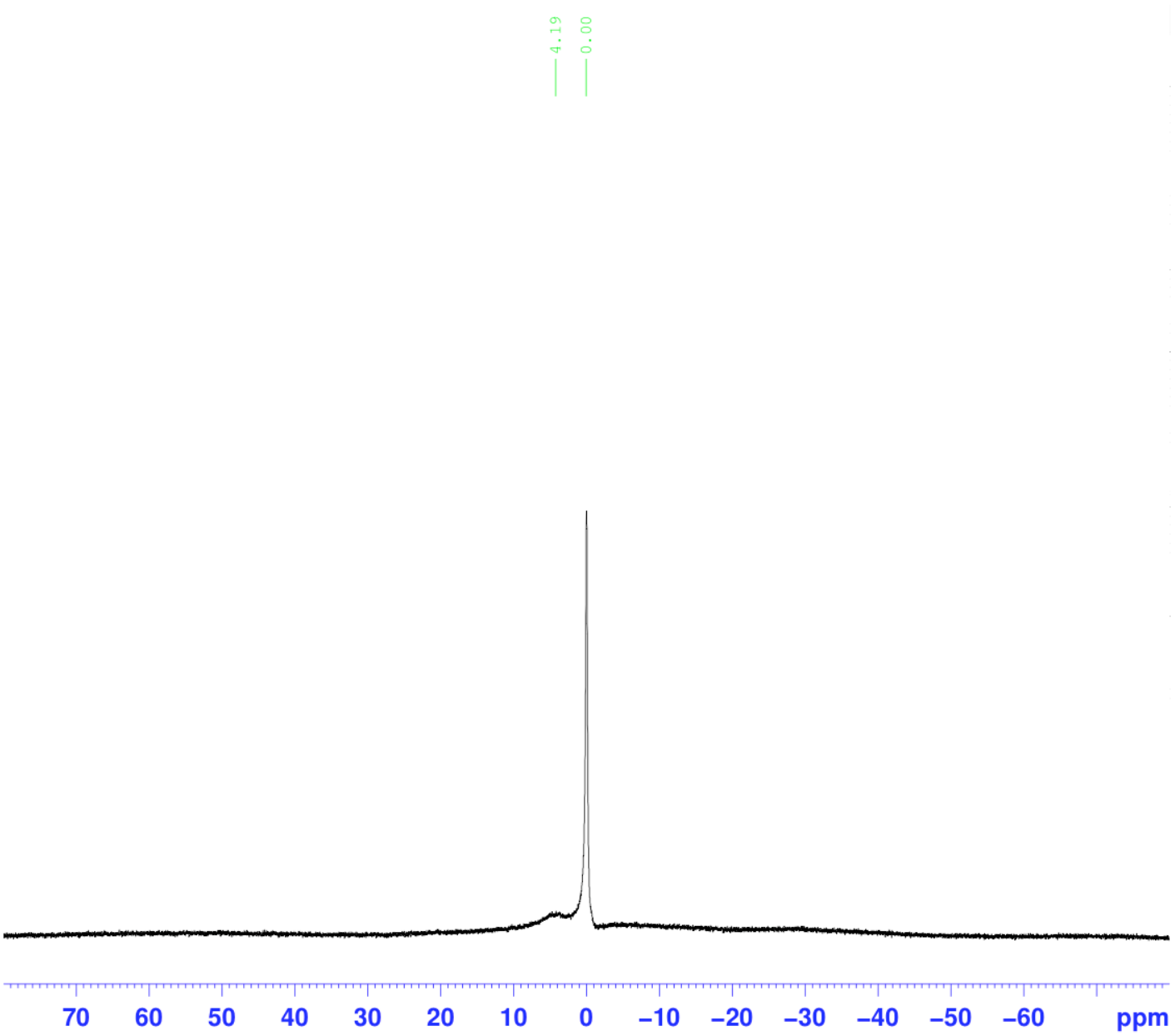
Aromatic region



1 + Et_3N

^{11} B NMR

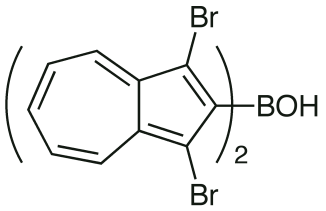
(128 MHz, THF-d_8)



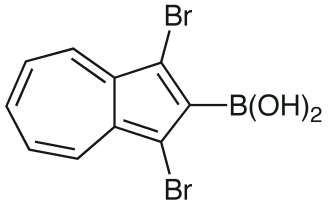
UV/Vis spectra of **1** and **6**
(in THF)

Blue line: **1**

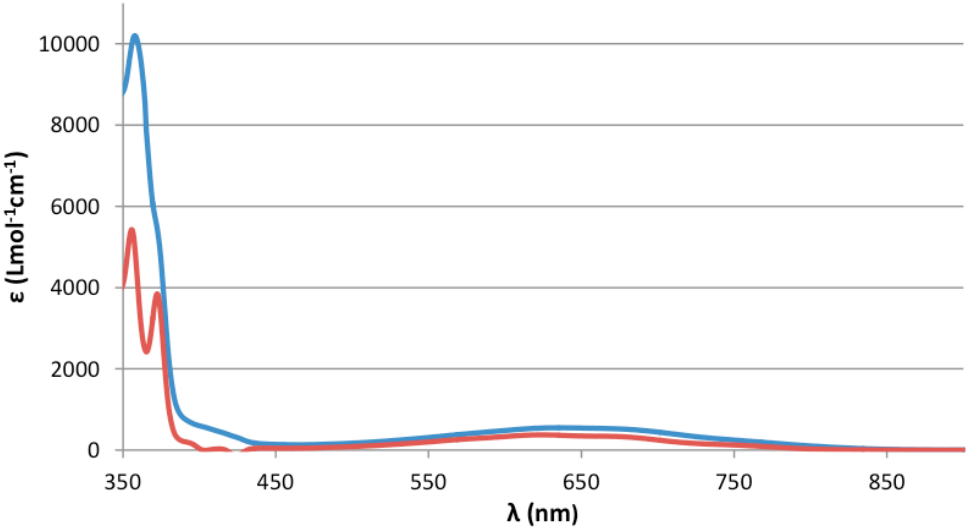
Red line: **6**

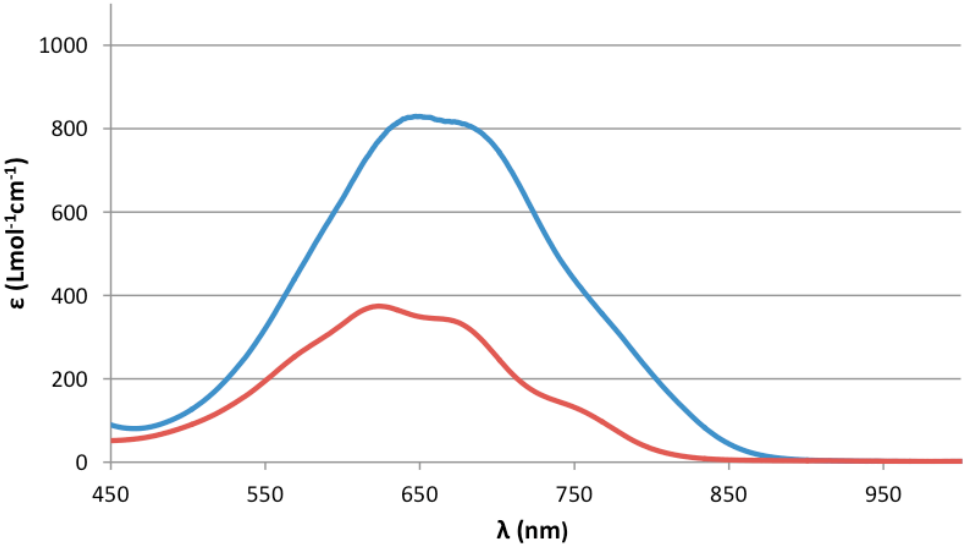


1



6





X-ray Structure Report

for

Compound 1

February 17, 2016

Experimental

Data Collection

A green unknown crystal of $C_{22}H_{15}BBr_4O_2$ having approximate dimensions of 0.200 x 0.200 x 0.060 mm was mounted on a glass fiber. All measurements were made on a Rigaku Mercury70 diffractometer using graphite monochromated Mo-Ka radiation.

The crystal-to-detector distance was 54.91 mm.

Cell constants and an orientation matrix for data collection corresponded to a C-centered monoclinic cell with dimensions:

a = 47.168(2) Å
b = 11.8390(4) Å b = 99.945(2)°
c = 15.7194(7) Å
V = 8646.1(6) Å^3

For Z = 16 and F.W. = 641.79, the calculated density is 1.972 g/cm^3. Based on the reflection conditions of:

hkl: h+k = 2n
h0l: l = 2n

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

C2/c (#15)

The data were collected at a temperature of -119 ± 1°C to a maximum 2θ value of 55.0°. A total of 1800 oscillation images were collected. A sweep of data was done using w scans from -65.0 to 115.0° in 0.30° step, at c=45.0° and f = 0.0°. The exposure rate was 100.0 [sec./°]. The detector swing angle was 24.96°. A second sweep was performed using w scans from -65.0 to 115.0° in 0.30° step, at c=45.0° and f = 90.0°. The exposure rate was 100.0 [sec./°]. The detector swing angle was 24.96°. Another sweep was performed using w scans from -65.0 to 115.0° in 0.30° step, at c=45.0° and f = 180.0°. The exposure rate was 100.0 [sec./°]. The detector swing angle was 24.96°. The crystal-to-detector distance was 54.91 mm. Readout was performed in the 0.137 mm pixel mode.

Data Reduction

Of the 42189 reflections were collected, where 9802 were unique (R_{int} = 0.0560); equivalent reflections were merged. Data were collected and processed using CrystalClear (Rigaku). [1]

The linear absorption coefficient, m, for Mo-Ka radiation is 74.862 cm^{-1}. A numerical absorption correction was applied which resulted in transmission factors ranging from 0.254 to 0.638. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 9802 observed reflections and 552 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = S \; ||Fo| - |Fc|| \; / \; S \; |Fo| = 0.0408$$

$$wR2 = [S (w (Fo^2 - Fc^2)^2) / S \; w(Fo^2)^2]^{1/2} = 0.1096$$

The goodness of fit[4] was 1.13. Unit weights were used. Plots of S w $(|Fo| - |Fc|)^2$ versus |Fo|, reflection order in data collection, sin q/l and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.47 and -1.07 e/$Å^3$, respectively.

Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4 [5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Df' and Df'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9] crystallographic software package except for refinement, which was performed using SHELXL97[10].

References

(1) CrystalClear: Data Collection and Processing Software, Rigaku Corporation (1998-2014). Tokyo 196-8666, Japan.

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C. and Guagliardi, A. (1993). J. Appl. Cryst. 26, 343-350.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Goodness of fit is defined as:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where: N_o = number of observations
N_v = number of variables

(5) International Tables for Crystallography, Vol.C (1992). Ed. A.J.C. Wilson, Kluwer Academic Publishers, Dordrecht, Netherlands, Table 6.1.1.4, pp. 572.

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 4.1: Crystal Structure Analysis Package, Rigaku Corporation (2000-2014). Tokyo 196-8666, Japan.

(10) SHELXL97: Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{22}H_{15}BBr_4O_2$
Formula Weight	641.79
Crystal Color, Habit	green, unknown
Crystal Dimensions	0.200 X 0.200 X 0.060 mm
Crystal System	monoclinic
Lattice Type	C-centered
Lattice Parameters	a = 47.168(2) Å b = 11.8390(4) Å c = 15.7194(7) Å b = 99.945(2) ^{o} V = 8646.1(6) Å^3
Space Group	C2/c (#15)
Z value	16
D_{calc}	1.972 g/cm^3
F_{000}	4928.00
m(MoKα)	74.862 cm^{-1}

B. Intensity Measurements

Diffractometer	Mercury70
Radiation	MoKα (l = 0.71075 Å) graphite monochromated
Voltage, Current	50kV, 40mA
Temperature	-119.8^{o}C
Detector Aperture	70.0 x 70.0 mm
Data Images	1800 exposures
w oscillation Range (c=45.0, f=0.0)	-65.0 - 115.0^{o}
Exposure Rate	100.0 sec./^{o}
Detector Swing Angle	24.96^{o}
w oscillation Range (c=45.0, f=90.0)	-65.0 - 115.0^{o}
Exposure Rate	100.0 sec./^{o}
Detector Swing Angle	24.96^{o}
w oscillation Range (c=45.0, f=180.0)	-65.0 - 115.0^{o}
Exposure Rate	100.0 sec./^{o}
Detector Swing Angle	24.96^{o}
Detector Position	54.91 mm
Pixel Size	0.137 mm

$2\theta_{max}$	55.0^{o}
No. of Reflections Measured	Total: 42189 Unique: 9802 (R_{int} = 0.0560)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.254 - 0.638)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma w (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0482 \cdot P)^2 + 2.9985 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	9802
No. Variables	552
Reflection/Parameter Ratio	17.76
Residuals: R1 ($I>2.00\sigma(I)$)	0.0408
Residuals: R (All reflections)	0.0498
Residuals: wR2 (All reflections)	0.1096
Goodness of Fit Indicator	1.128
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.47 e/$Å^3$
Minimum peak in Final Diff. Map	-1.07 e/$Å^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Br1	0.475260(9)	0.97402(4)	0.64503(3)	2.830(9)	1
Br2	0.384121(9)	0.63950(3)	0.56328(3)	2.941(10)	1
Br3	0.427434(9)	0.54492(3)	0.85621(3)	2.992(10)	1
Br4	0.370001(8)	0.93416(3)	0.67517(2)	2.341(8)	1
Br5	0.345722(10)	1.44697(3)	0.70141(3)	3.084(10)	1
Br6	0.295378(8)	1.05678(3)	0.50750(3)	2.587(9)	1
Br7	0.330185(8)	1.11747(3)	0.79560(2)	2.427(8)	1
Br8	0.245764(8)	1.48149(3)	0.73223(2)	2.483(9)	1
O1	0.45848(6)	0.7725(2)	0.76707(17)	2.64(5)	1
O2	0.26058(6)	1.2737(3)	0.59489(19)	4.09(7)	1
O3	0.52162(7)	0.7552(3)	0.5560(2)	3.56(6)	1
O4	0.48977(17)	0.6669(7)	0.4556(6)	4.18(18)	0.450000
O5	0.48500(12)	0.6328(4)	0.5300(4)	3.09(10)	0.550000
C1	0.44684(8)	0.8792(3)	0.5846(2)	1.94(6)	1
C2	0.42979(7)	0.8024(3)	0.6224(2)	1.94(6)	1
C3	0.41124(8)	0.7526(3)	0.5522(2)	1.98(6)	1
C4	0.40255(9)	0.7621(3)	0.3912(2)	2.64(7)	1
C5	0.40651(10)	0.8023(4)	0.3110(3)	3.29(8)	1
C6	0.42540(10)	0.8843(4)	0.2923(3)	3.40(8)	1
C7	0.44514(9)	0.9490(4)	0.3477(3)	2.95(8)	1
C8	0.45167(8)	0.9467(3)	0.4374(3)	2.29(6)	1
C9	0.43966(8)	0.8796(3)	0.4939(2)	1.97(6)	1
C10	0.41630(8)	0.7933(3)	0.4728(2)	2.10(6)	1
C11	0.40005(8)	0.6582(3)	0.8172(2)	1.99(6)	1
C12	0.40422(8)	0.7473(3)	0.7614(2)	1.96(6)	1
C13	0.37772(8)	0.8059(3)	0.7471(2)	1.78(6)	1
C14	0.32905(8)	0.7884(3)	0.7878(2)	2.17(6)	1
C15	0.30801(9)	0.7388(3)	0.8273(3)	2.68(7)	1
C16	0.31014(8)	0.6450(3)	0.8814(3)	2.59(7)	1
C17	0.33355(9)	0.5751(3)	0.9090(2)	2.44(7)	1
C18	0.36118(8)	0.5809(3)	0.8890(2)	2.16(6)	1
C19	0.37221(8)	0.6568(3)	0.8366(2)	1.89(6)	1
C20	0.35735(8)	0.7557(3)	0.7895(2)	1.97(6)	1
C21	0.34080(8)	1.3198(3)	0.6285(2)	2.09(6)	1
C22	0.31491(8)	1.2573(3)	0.6085(2)	1.79(6)	1
C23	0.32117(7)	1.1717(3)	0.5528(2)	1.79(6)	1
C24	0.36244(8)	1.1046(3)	0.4875(2)	2.02(6)	1

Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C25	0.39041(9)	1.1058(3)	0.4707(3)	2.55(7)	1
C26	0.41224(8)	1.1817(4)	0.4997(3)	2.98(8)	1
C27	0.41221(9)	1.2747(4)	0.5531(3)	3.21(8)	1
C28	0.39001(8)	1.3177(3)	0.5920(2)	2.45(7)	1
C29	0.36259(8)	1.2763(3)	0.5879(2)	1.82(6)	1
C30	0.34933(7)	1.1769(3)	0.5381(2)	1.76(6)	1
C31	0.30445(8)	1.2341(3)	0.8125(2)	1.97(6)	1
C32	0.28745(7)	1.2947(3)	0.7454(2)	1.92(6)	1
C33	0.27134(8)	1.3702(3)	0.7877(2)	1.86(6)	1
C34	0.26566(8)	1.4198(3)	0.9374(2)	2.48(7)	1
C35	0.27131(9)	1.4128(4)	1.0268(3)	2.96(8)	1
C36	0.29020(10)	1.3409(4)	1.0783(3)	3.13(8)	1
C37	0.30883(9)	1.2597(4)	1.0555(3)	3.07(8)	1
C38	0.31303(8)	1.2275(3)	0.9734(2)	2.30(6)	1
C39	0.29962(7)	1.2683(3)	0.8941(2)	1.79(6)	1
C40	0.27755(7)	1.3589(3)	0.8770(2)	1.76(6)	1
C41	0.5032(3)	0.7060(10)	0.5011(8)	3.3(2)	0.550000
C42	0.5024(3)	0.6898(12)	0.5385(9)	2.6(2)	0.450000
C43	0.49949(13)	0.7308(5)	0.4010(3)	4.58(11)	1
C44	0.48873(11)	0.6145(4)	0.6160(4)	4.32(10)	1
C45	0.4839(3)	0.7022(10)	0.3089(7)	5.4(3)	0.450000
C46	0.46406(18)	0.5306(7)	0.6326(7)	4.4(2)	0.550000
B1	0.43161(9)	0.7741(3)	0.7210(3)	2.12(7)	1
B2	0.28654(9)	1.2767(4)	0.6460(3)	2.05(7)	1

$B_{eq} = 8/3\ p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

Table 2. Atomic coordinates and B_{iso} involving hydrogen atoms

atom	x	y	z	B_{iso}	occ
H1	0.45776	0.75863	0.81906	3.167	1
H2	0.26094	1.31311	0.55067	4.913	1
H4	0.38835	0.70492	0.38976	3.172	1
H5	0.39466	0.76900	0.26250	3.948	1
H6	0.42479	0.89861	0.23257	4.082	1
H7	0.45565	1.00235	0.32043	3.541	1
H8	0.46622	0.99768	0.46311	2.754	1
H14	0.32320	0.85430	0.75484	2.603	1
H15	0.28960	0.77362	0.81570	3.217	1
H16	0.29307	0.62612	0.90265	3.113	1
H17	0.33032	0.51532	0.94655	2.923	1
H18	0.37424	0.52469	0.91507	2.594	1
H24	0.35058	1.04551	0.46023	2.429	1
H25	0.39515	1.04691	0.43457	3.066	1
H26	0.42988	1.16794	0.48004	3.574	1
H27	0.42985	1.31516	0.56507	3.855	1
H28	0.39443	1.38412	0.62559	2.937	1
H34	0.25163	1.47425	0.91424	2.980	1
H35	0.26092	1.46365	1.05659	3.555	1
H36	0.29045	1.34827	1.13856	3.757	1
H37	0.32021	1.22093	1.10226	3.679	1
H38	0.32696	1.17003	0.97157	2.757	1

Table 3. Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Br1	0.0357(2)	0.0433(2)	0.0296(2)	-0.01619(17)	0.00854(18)	-0.00551(17)
Br2	0.0413(2)	0.0378(2)	0.0342(2)	-0.01716(17)	0.01086(19)	-0.00768(17)
Br3	0.0332(2)	0.0333(2)	0.0482(3)	0.00610(16)	0.01010(19)	0.01371(18)
Br4	0.0344(2)	0.02508(19)	0.0301(2)	0.00226(14)	0.00741(17)	0.00549(15)
Br5	0.0474(3)	0.0336(2)	0.0380(3)	-0.00871(17)	0.0126(2)	-0.01510(17)
Br6	0.0268(2)	0.0343(2)	0.0380(2)	-0.00694(15)	0.00783(17)	-0.01052(16)
Br7	0.0324(2)	0.0305(2)	0.0305(2)	0.01012(15)	0.00860(17)	-0.00050(15)
Br8	0.0328(2)	0.0384(2)	0.0232(2)	0.01257(16)	0.00495(16)	0.00244(16)
O1	0.0310(14)	0.0451(16)	0.0250(14)	-0.0021(12)	0.0074(11)	0.0066(13)
O2	0.0360(17)	0.087(3)	0.0288(17)	0.0208(17)	-0.0037(13)	-0.0176(17)
O3	0.0409(18)	0.0474(18)	0.0465(19)	-0.0081(14)	0.0064(15)	-0.0036(15)
O4	0.039(4)	0.049(5)	0.065(6)	0.002(3)	-0.009(4)	-0.027(5)
O5	0.036(3)	0.035(3)	0.044(4)	0.004(3)	0.001(3)	-0.006(3)
C1	0.0255(18)	0.0252(17)	0.0236(19)	-0.0013(14)	0.0061(15)	-0.0039(14)
C2	0.0240(18)	0.0242(17)	0.0267(19)	-0.0023(14)	0.0075(15)	-0.0020(14)
C3	0.0257(18)	0.0244(17)	0.0263(19)	-0.0028(14)	0.0072(15)	-0.0025(14)
C4	0.031(2)	0.041(2)	0.028(2)	-0.0010(17)	0.0020(17)	-0.0076(17)
C5	0.039(2)	0.059(3)	0.024(2)	0.001(2)	-0.0017(18)	-0.003(2)
C6	0.043(3)	0.063(3)	0.024(2)	0.010(2)	0.0077(19)	0.012(2)
C7	0.038(2)	0.044(2)	0.032(2)	0.0004(18)	0.0110(19)	0.0089(19)
C8	0.0239(19)	0.0325(19)	0.032(2)	0.0012(14)	0.0095(16)	0.0034(16)
C9	0.0228(18)	0.0270(18)	0.027(2)	0.0024(14)	0.0091(15)	0.0004(15)
C10	0.0254(18)	0.0287(18)	0.026(2)	0.0036(14)	0.0053(15)	-0.0009(15)
C11	0.0272(19)	0.0248(17)	0.0240(19)	-0.0012(14)	0.0053(15)	0.0045(14)
C12	0.0297(19)	0.0253(17)	0.0185(18)	-0.0001(14)	0.0010(15)	-0.0010(14)
C13	0.0274(18)	0.0221(16)	0.0180(18)	0.0012(14)	0.0033(14)	-0.0008(13)
C14	0.0290(19)	0.0312(19)	0.0235(19)	0.0015(15)	0.0081(16)	-0.0048(15)
C15	0.030(2)	0.038(2)	0.034(2)	-0.0023(17)	0.0065(17)	-0.0075(18)
C16	0.029(2)	0.040(2)	0.031(2)	-0.0091(16)	0.0079(17)	-0.0034(17)
C17	0.040(2)	0.0286(19)	0.026(2)	-0.0094(16)	0.0098(17)	-0.0007(15)
C18	0.035(2)	0.0256(18)	0.0214(19)	-0.0019(15)	0.0051(16)	-0.0019(15)
C19	0.0282(19)	0.0259(17)	0.0178(18)	-0.0010(14)	0.0042(14)	-0.0029(14)
C20	0.033(2)	0.0259(17)	0.0170(18)	-0.0012(15)	0.0067(15)	-0.0039(14)
C21	0.031(2)	0.0250(17)	0.0249(19)	-0.0008(14)	0.0076(16)	-0.0038(15)
C22	0.0273(18)	0.0236(17)	0.0173(17)	-0.0003(14)	0.0048(14)	0.0005(14)
C23	0.0239(18)	0.0274(17)	0.0168(17)	-0.0011(14)	0.0034(14)	0.0005(14)
C24	0.0255(19)	0.0274(18)	0.0245(19)	0.0053(14)	0.0057(15)	0.0021(15)

Table 3. Anisotropic displacement parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C25	0.035(2)	0.033(2)	0.032(2)	0.0112(17)	0.0148(18)	0.0047(17)
C26	0.025(2)	0.044(2)	0.045(3)	0.0084(17)	0.0099(18)	0.010(2)
C27	0.024(2)	0.053(3)	0.045(3)	-0.0042(18)	0.0050(18)	0.010(2)
C28	0.032(2)	0.033(2)	0.027(2)	-0.0047(16)	0.0028(17)	0.0036(16)
C29	0.0256(18)	0.0255(17)	0.0172(17)	0.0014(14)	0.0008(14)	0.0024(14)
C30	0.0239(18)	0.0242(17)	0.0192(18)	0.0000(13)	0.0044(14)	0.0028(14)
C31	0.0239(18)	0.0248(17)	0.0272(19)	0.0027(14)	0.0076(15)	-0.0022(15)
C32	0.0214(17)	0.0279(18)	0.0247(19)	0.0008(14)	0.0072(14)	-0.0004(15)
C33	0.0227(17)	0.0274(18)	0.0216(18)	0.0031(14)	0.0068(14)	-0.0016(14)
C34	0.030(2)	0.040(2)	0.025(2)	0.0096(16)	0.0072(16)	-0.0008(17)
C35	0.040(2)	0.051(3)	0.023(2)	0.014(2)	0.0104(18)	-0.0027(19)
C36	0.044(3)	0.053(3)	0.022(2)	0.007(2)	0.0046(18)	-0.0015(19)
C37	0.044(3)	0.043(2)	0.028(2)	0.0107(19)	0.0010(19)	0.0043(18)
C38	0.033(2)	0.0281(19)	0.026(2)	0.0050(15)	0.0037(16)	0.0045(16)
C39	0.0204(17)	0.0248(17)	0.0238(18)	-0.0012(13)	0.0063(14)	-0.0014(14)
C40	0.0204(17)	0.0263(17)	0.0210(18)	-0.0004(13)	0.0059(14)	0.0010(14)
C41	0.059(7)	0.031(5)	0.042(8)	0.011(5)	0.031(7)	0.003(5)
C42	0.021(5)	0.037(7)	0.046(9)	0.002(4)	0.021(6)	-0.006(6)
C43	0.067(4)	0.062(3)	0.044(3)	0.011(3)	0.006(3)	-0.009(3)
C44	0.045(3)	0.042(3)	0.076(4)	0.002(2)	0.007(3)	0.007(3)
C45	0.091(10)	0.058(7)	0.050(7)	0.022(7)	-0.006(7)	-0.010(6)
C46	0.025(4)	0.050(5)	0.086(7)	-0.007(3)	-0.001(4)	0.028(5)
B1	0.032(2)	0.0229(19)	0.026(2)	0.0006(16)	0.0074(18)	0.0005(17)
B2	0.027(2)	0.029(2)	0.023(2)	0.0052(16)	0.0084(17)	-0.0006(17)

The general temperature factor expression: $\exp(-2p^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table 4. Fragment Analysis

fragment: 1

Br(1)	Br(2)	Br(3)	Br(4)	O(1)
C(1)	C(2)	C(3)	C(4)	C(5)
C(6)	C(7)	C(8)	C(9)	C(10)
C(11)	C(12)	C(13)	C(14)	C(15)
C(16)	C(17)	C(18)	C(19)	C(20)
B(1)				

fragment: 2

Br(5)	Br(6)	Br(7)	Br(8)	O(2)
C(21)	C(22)	C(23)	C(24)	C(25)
C(26)	C(27)	C(28)	C(29)	C(30)
C(31)	C(32)	C(33)	C(34)	C(35)
C(36)	C(37)	C(38)	C(39)	C(40)
B(2)				

fragment: 3

O(3)	O(4)	O(5)	C(41)	C(42)
C(43)	C(44)	C(45)	C(46)	

Table 5. Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Br1	C1	1.876(3)	Br2	C3	1.880(4)
Br3	C11	1.889(3)	Br4	C13	1.891(3)
Br5	C21	1.882(3)	Br6	C23	1.882(3)
Br7	C31	1.887(4)	Br8	C33	1.895(3)
O1	B1	1.347(5)	O2	B2	1.344(5)
O3	C41	1.257(13)	O3	C42	1.187(13)
O4	O5	1.294(11)	O4	C41	0.985(15)
O4	C42	1.364(16)	O4	C43	1.287(11)
O5	C41	1.353(15)	O5	C42	1.054(14)
O5	C44	1.350(8)	C1	C2	1.412(5)
C1	C9	1.408(5)	C2	C3	1.414(5)
C2	B1	1.573(6)	C3	C10	1.396(5)
C4	C5	1.390(6)	C4	C10	1.384(5)
C5	C6	1.383(7)	C6	C7	1.390(6)
C7	C8	1.390(6)	C8	C9	1.384(6)
C9	C10	1.497(5)	C11	C12	1.407(5)
C11	C19	1.398(6)	C12	C13	1.413(5)
C12	B1	1.567(6)	C13	C20	1.394(5)
C14	C15	1.389(6)	C14	C20	1.386(5)
C15	C16	1.392(6)	C16	C17	1.388(5)
C17	C18	1.394(6)	C18	C19	1.381(5)
C19	C20	1.493(5)	C21	C22	1.416(5)
C21	C29	1.398(6)	C22	C23	1.403(5)
C22	B2	1.570(6)	C23	C30	1.388(5)
C24	C25	1.389(6)	C24	C30	1.386(5)
C25	C26	1.383(6)	C26	C27	1.386(6)
C27	C28	1.396(6)	C28	C29	1.374(5)
C29	C30	1.490(5)	C31	C32	1.407(5)
C31	C39	1.401(5)	C32	C33	1.412(5)
C32	B2	1.570(6)	C33	C40	1.390(5)
C34	C35	1.387(5)	C34	C40	1.385(5)
C35	C36	1.387(6)	C36	C37	1.390(6)
C37	C38	1.392(6)	C38	C39	1.383(5)
C39	C40	1.486(5)	C41	C42	0.63(2)
C41	C43	1.580(13)	C42	C44	1.723(16)
C43	C45	1.544(12)	C44	C46	1.585(10)

Table 6. Bond lengths involving hydrogens (Å)

atom	atom	distance	atom	atom	distance
O1	H1	0.840	O2	H2	0.840
C4	H4	0.950	C5	H5	0.950
C6	H6	0.950	C7	H7	0.950
C8	H8	0.950	C14	H14	0.950
C15	H15	0.950	C16	H16	0.950
C17	H17	0.950	C18	H18	0.950
C24	H24	0.950	C25	H25	0.950
C26	H26	0.950	C27	H27	0.950
C28	H28	0.950	C34	H34	0.950
C35	H35	0.950	C36	H36	0.950
C37	H37	0.950	C38	H38	0.950

Table 7. Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C41	O3	C42	29.5(9)	O5	O4	C41	71.4(10)
O5	O4	C42	46.6(7)	O5	O4	C43	157.6(8)
C41	O4	C42	24.8(10)	C41	O4	C43	87.1(10)
C42	O4	C43	111.9(9)	O4	O5	C41	43.6(6)
O4	O5	C42	70.2(9)	O4	O5	C44	160.5(6)
C41	O5	C42	26.6(9)	C41	O5	C44	117.3(7)
C42	O5	C44	90.7(9)	Br1	C1	C2	125.6(3)
Br1	C1	C9	122.5(3)	C2	C1	C9	112.0(3)
C1	C2	C3	105.1(3)	C1	C2	B1	127.9(3)
C3	C2	B1	127.0(3)	Br2	C3	C2	124.3(3)
Br2	C3	C10	123.5(3)	C2	C3	C10	112.1(3)
C5	C4	C10	129.4(4)	C4	C5	C6	128.7(4)
C5	C6	C7	129.8(4)	C6	C7	C8	129.2(4)
C7	C8	C9	128.2(3)	C1	C9	C8	126.8(3)
C1	C9	C10	105.1(3)	C8	C9	C10	128.1(3)
C3	C10	C4	127.7(4)	C3	C10	C9	105.7(3)
C4	C10	C9	126.6(4)	Br3	C11	C12	125.0(3)
Br3	C11	C19	122.4(3)	C12	C11	C19	112.4(3)
C11	C12	C13	104.6(3)	C11	C12	B1	128.1(3)
C13	C12	B1	127.2(3)	Br4	C13	C12	124.3(3)
Br4	C13	C20	123.4(3)	C12	C13	C20	112.3(3)
C15	C14	C20	129.3(3)	C14	C15	C16	129.0(4)
C15	C16	C17	129.5(4)	C16	C17	C18	128.6(4)
C17	C18	C19	129.0(3)	C11	C19	C18	127.0(3)
C11	C19	C20	105.1(3)	C18	C19	C20	127.8(4)
C13	C20	C14	127.8(3)	C13	C20	C19	105.5(3)
C14	C20	C19	126.7(3)	Br5	C21	C22	124.3(3)
Br5	C21	C29	123.3(3)	C22	C21	C29	112.3(3)
C21	C22	C23	104.4(3)	C21	C22	B2	126.8(3)
C23	C22	B2	128.7(3)	Br6	C23	C22	124.5(3)
Br6	C23	C30	122.9(3)	C22	C23	C30	112.5(3)
C25	C24	C30	129.4(3)	C24	C25	C26	128.4(4)
C25	C26	C27	129.6(4)	C26	C27	C28	129.4(4)
C27	C28	C29	128.3(4)	C21	C29	C28	127.4(3)
C21	C29	C30	104.8(3)	C28	C29	C30	127.8(3)
C23	C30	C24	127.1(3)	C23	C30	C29	105.9(3)
C24	C30	C29	127.0(3)	Br7	C31	C32	124.4(3)

Table 7. Bond angles (^{o}) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Br7	C31	C39	123.4(2)	C32	C31	C39	112.2(3)
C31	C32	C33	104.7(3)	C31	C32	B2	126.2(3)
C33	C32	B2	129.1(3)	Br8	C33	C32	125.1(3)
Br8	C33	C40	122.6(3)	C32	C33	C40	112.2(3)
C35	C34	C40	129.3(4)	C34	C35	C36	128.3(4)
C35	C36	C37	130.2(4)	C36	C37	C38	128.7(4)
C37	C38	C39	128.6(4)	C31	C39	C38	127.1(3)
C31	C39	C40	105.2(3)	C38	C39	C40	127.7(3)
C33	C40	C34	127.0(3)	C33	C40	C39	105.7(3)
C34	C40	C39	127.3(3)	O3	C41	O4	176.1(17)
O3	C41	O5	118.0(10)	O3	C41	C42	69.0(16)
O3	C41	C43	122.8(10)	O4	C41	O5	65.0(10)
O4	C41	C42	114(2)	O4	C41	C43	54.4(8)
O5	C41	C42	49.0(16)	O5	C41	C43	119.1(9)
C42	C41	C43	168(2)	O3	C42	O4	122.7(12)
O3	C42	O5	173.7(16)	O3	C42	C41	81.5(18)
O3	C42	C44	122.6(10)	O4	C42	O5	63.2(8)
O4	C42	C41	41.3(15)	O4	C42	C44	114.7(9)
O5	C42	C41	104(2)	O5	C42	C44	51.6(7)
C41	C42	C44	156(2)	O4	C43	C41	38.5(6)
O4	C43	C45	109.2(7)	C41	C43	C45	147.7(8)
O5	C44	C42	37.7(5)	O5	C44	C46	107.0(5)
C42	C44	C46	144.7(7)	O1	B1	C2	114.7(4)
O1	B1	C12	123.0(3)	C2	B1	C12	122.3(3)
O2	B2	C22	121.3(3)	O2	B2	C32	117.7(4)
C22	B2	C32	121.0(3)				

Table 8. Bond angles involving hydrogens (°)

atom	atom	atom	angle	atom	atom	atom	angle
B1	O1	H1	109.5	B2	O2	H2	109.5
C5	C4	H4	115.3	C10	C4	H4	115.3
C4	C5	H5	115.7	C6	C5	H5	115.6
C5	C6	H6	115.1	C7	C6	H6	115.1
C6	C7	H7	115.4	C8	C7	H7	115.4
C7	C8	H8	115.9	C9	C8	H8	115.9
C15	C14	H14	115.4	C20	C14	H14	115.4
C14	C15	H15	115.5	C16	C15	H15	115.5
C15	C16	H16	115.2	C17	C16	H16	115.2
C16	C17	H17	115.7	C18	C17	H17	115.7
C17	C18	H18	115.5	C19	C18	H18	115.5
C25	C24	H24	115.3	C30	C24	H24	115.3
C24	C25	H25	115.8	C26	C25	H25	115.8
C25	C26	H26	115.2	C27	C26	H26	115.2
C26	C27	H27	115.3	C28	C27	H27	115.3
C27	C28	H28	115.8	C29	C28	H28	115.8
C35	C34	H34	115.4	C40	C34	H34	115.4
C34	C35	H35	115.9	C36	C35	H35	115.8
C35	C36	H36	114.9	C37	C36	H36	114.9
C36	C37	H37	115.6	C38	C37	H37	115.7
C37	C38	H38	115.7	C39	C38	H38	115.7

Table 9. Torsion Angles(O)
(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C41	O3	C42	O4	2.3(13)	C41	O3	C42	C41	0.0(13)
C41	O3	C42	C44	-179(2)	C42	O3	C41	O5	2.0(13)
C42	O3	C41	C42	-0.0(13)	C42	O3	C41	C43	179(2)
O5	O4	C41	O5	0.0(3)	O5	O4	C41	C42	4.4(16)
O5	O4	C41	C43	-173.8(7)	C41	O4	O5	C41	0.0(8)
C41	O4	O5	C42	-2.5(9)	O5	O4	C42	O3	-177.7(17)
O5	O4	C42	O5	-0.0(3)	O5	O4	C42	C41	-174.3(19)
O5	O4	C42	C44	3.4(5)	C42	O4	O5	C41	2.5(8)
C42	O4	O5	C42	0.0(8)	O5	O4	C43	C41	15.6(16)
O5	O4	C43	C45	-164.0(18)	C43	O4	O5	C41	-16.5(17)
C43	O4	O5	C42	-19(2)	C41	O4	C42	O3	-3(2)
C41	O4	C42	O5	174(3)	C41	O4	C42	C41	-0.0(19)
C41	O4	C42	C44	178(3)	C42	O4	C41	O5	-4(2)
C42	O4	C41	C42	-0.0(13)	C42	O4	C41	C43	-178(2)
C41	O4	C43	C41	0.0(8)	C41	O4	C43	C45	-179.6(9)
C43	O4	C41	O5	173.8(7)	C43	O4	C41	C42	178.2(18)
C43	O4	C41	C43	0.0(3)	C42	O4	C43	C41	0.8(6)
C42	O4	C43	C45	-178.8(8)	C43	O4	C42	O3	-5.4(16)
C43	O4	C42	O5	172.3(8)	C43	O4	C42	C41	-2.0(15)
C43	O4	C42	C44	175.7(7)	O4	O5	C41	O3	-177.2(17)
O4	O5	C41	O4	0.0(5)	O4	O5	C41	C42	-174.7(19)
O4	O5	C41	C43	5.8(6)	O4	O5	C42	O4	-0.0(4)
O4	O5	C42	C41	3.9(13)	O4	O5	C42	C44	-176.1(6)
C41	O5	C42	O4	-3.9(18)	C41	O5	C42	C41	-0.0(13)
C41	O5	C42	C44	-180(2)	C42	O5	C41	O3	-2.5(17)
C42	O5	C41	O4	175(2)	C42	O5	C41	C42	0.0(16)
C42	O5	C41	C43	-180(3)	C41	O5	C44	C42	0.0(7)
C41	O5	C44	C46	177.5(7)	C44	O5	C41	O3	-2.5(14)
C44	O5	C41	O4	174.7(6)	C44	O5	C41	C42	-0.0(15)
C44	O5	C41	C43	-179.5(7)	C42	O5	C44	C42	-0.0(7)
C42	O5	C44	C46	177.5(8)	C44	O5	C42	O4	176.1(5)
C44	O5	C42	C41	180.0(15)	C44	O5	C42	C44	0.0(2)
Br1	C1	C2	C3	178.6(2)	Br1	C1	C2	B1	-3.5(5)
Br1	C1	C9	C8	-0.3(5)	Br1	C1	C9	C10	-179.7(2)
C2	C1	C9	C8	178.3(3)	C2	C1	C9	C10	-1.1(4)
C9	C1	C2	C3	0.1(4)	C9	C1	C2	B1	178.0(3)
C1	C2	C3	Br2	178.2(3)	C1	C2	C3	C10	1.0(4)

Table 9. Torsion angles (°) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	C2	B1	O1	-36.9(5)	C1	C2	B1	C12	144.4(3)
C3	C2	B1	O1	140.6(3)	C3	C2	B1	C12	-38.2(5)
B1	C2	C3	Br2	0.3(5)	B1	C2	C3	C10	-176.9(3)
Br2	C3	C10	C4	1.7(5)	Br2	C3	C10	C9	-178.9(2)
C2	C3	C10	C4	178.9(3)	C2	C3	C10	C9	-1.7(4)
C5	C4	C10	C3	178.4(4)	C5	C4	C10	C9	-0.9(7)
C10	C4	C5	C6	0.1(8)	C4	C5	C6	C7	-0.7(8)
C5	C6	C7	C8	1.6(8)	C6	C7	C8	C9	-0.9(7)
C7	C8	C9	C1	179.8(4)	C7	C8	C9	C10	-0.9(6)
C1	C9	C10	C3	1.7(4)	C1	C9	C10	C4	-178.9(3)
C8	C9	C10	C3	-177.7(3)	C8	C9	C10	C4	1.7(6)
Br3	C11	C12	C13	177.0(2)	Br3	C11	C12	B1	-1.0(5)
Br3	C11	C19	C18	4.2(5)	Br3	C11	C19	C20	-176.59(19)
C12	C11	C19	C18	179.9(3)	C12	C11	C19	C20	-0.9(4)
C19	C11	C12	C13	1.4(4)	C19	C11	C12	B1	-176.6(3)
C11	C12	C13	Br4	-179.1(2)	C11	C12	C13	C20	-1.4(4)
C11	C12	B1	O1	-45.6(5)	C11	C12	B1	C2	133.1(3)
C13	C12	B1	O1	136.9(3)	C13	C12	B1	C2	-44.5(5)
B1	C12	C13	Br4	-1.1(5)	B1	C12	C13	C20	176.6(3)
Br4	C13	C20	C14	-0.3(5)	Br4	C13	C20	C19	178.62(19)
C12	C13	C20	C14	-178.0(3)	C12	C13	C20	C19	0.9(4)
C15	C14	C20	C13	178.0(3)	C15	C14	C20	C19	-0.6(6)
C20	C14	C15	C16	2.4(7)	C14	C15	C16	C17	-1.4(7)
C15	C16	C17	C18	-0.2(7)	C16	C17	C18	C19	-0.4(6)
C17	C18	C19	C11	-178.9(3)	C17	C18	C19	C20	2.1(6)
C11	C19	C20	C13	-0.0(3)	C11	C19	C20	C14	178.9(3)
C18	C19	C20	C13	179.2(3)	C18	C19	C20	C14	-1.9(6)
Br5	C21	C22	C23	179.9(2)	Br5	C21	C22	B2	-3.6(5)
Br5	C21	C29	C28	-1.5(5)	Br5	C21	C29	C30	179.6(2)
C22	C21	C29	C28	178.6(3)	C22	C21	C29	C30	-0.3(4)
C29	C21	C22	C23	-0.2(4)	C29	C21	C22	B2	176.3(3)
C21	C22	C23	Br6	177.3(2)	C21	C22	C23	C30	0.7(4)
C21	C22	B2	O2	136.6(4)	C21	C22	B2	C32	-46.2(5)
C23	C22	B2	O2	-47.8(5)	C23	C22	B2	C32	129.4(3)
B2	C22	C23	Br6	0.9(5)	B2	C22	C23	C30	-175.7(3)
Br6	C23	C30	C24	2.6(5)	Br6	C23	C30	C29	-177.54(19)
C22	C23	C30	C24	179.2(3)	C22	C23	C30	C29	-0.9(4)

Table 9. Torsion angles (^{o}) (continued)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C25	C24	C30	C23	-180.0(3)	C25	C24	C30	C29	0.1(6)
C30	C24	C25	C26	-1.1(7)	C24	C25	C26	C27	0.7(7)
C25	C26	C27	C28	-0.4(7)	C26	C27	C28	C29	1.4(7)
C27	C28	C29	C21	178.9(3)	C27	C28	C29	C30	-2.4(6)
C21	C29	C30	C23	0.7(3)	C21	C29	C30	C24	-179.4(3)
C28	C29	C30	C23	-178.2(3)	C28	C29	C30	C24	1.7(6)
Br7	C31	C32	C33	178.6(2)	Br7	C31	C32	B2	0.5(5)
Br7	C31	C39	C38	2.5(5)	Br7	C31	C39	C40	-178.6(2)
C32	C31	C39	C38	-178.9(3)	C32	C31	C39	C40	-0.0(4)
C39	C31	C32	C33	0.0(4)	C39	C31	C32	B2	-178.1(3)
C31	C32	C33	Br8	176.3(3)	C31	C32	C33	C40	-0.1(4)
C31	C32	B2	O2	134.8(4)	C31	C32	B2	C22	-42.5(5)
C33	C32	B2	O2	-43.0(5)	C33	C32	B2	C22	139.8(3)
B2	C32	C33	Br8	-5.6(5)	B2	C32	C33	C40	178.0(3)
Br8	C33	C40	C34	3.4(5)	Br8	C33	C40	C39	-176.4(2)
C32	C33	C40	C34	179.9(3)	C32	C33	C40	C39	0.1(4)
C35	C34	C40	C33	-179.2(4)	C35	C34	C40	C39	0.6(6)
C40	C34	C35	C36	-1.0(7)	C34	C35	C36	C37	1.8(8)
C35	C36	C37	C38	-1.3(8)	C36	C37	C38	C39	-0.2(7)
C37	C38	C39	C31	179.8(3)	C37	C38	C39	C40	1.2(6)
C31	C39	C40	C33	-0.0(3)	C31	C39	C40	C34	-179.8(3)
C38	C39	C40	C33	178.8(3)	C38	C39	C40	C34	-1.0(6)
O3	C41	C42	O3	-0.00(16)	O3	C41	C42	O4	-177.1(16)
O3	C41	C42	O5	177.6(16)	O3	C41	C42	C44	178(5)
O3	C41	C43	O4	176.7(17)	O3	C41	C43	C45	177.3(7)
O4	C41	C42	O3	177.1(17)	O4	C41	C42	O4	0.0(5)
O4	C41	C42	O5	-5(2)	O4	C41	C42	C44	-5(6)
O4	C41	C43	O4	0.0(6)	O4	C41	C43	C45	0.7(17)
O5	C41	C42	O3	-177.6(16)	O5	C41	C42	O4	5(2)
O5	C41	C42	O5	0.0(3)	O5	C41	C42	C44	0(4)
O5	C41	C43	O4	-6.4(5)	O5	C41	C43	C45	-6(2)
O3	C42	C44	O5	177.2(17)	O3	C42	C44	C46	173.1(6)
O4	C42	C44	O5	-3.8(5)	O4	C42	C44	C46	-7.9(16)
O5	C42	C44	O5	0.0(4)	O5	C42	C44	C46	-4.1(14)
C41	C42	C44	O5	-0(5)	C41	C42	C44	C46	-4(6)

Table 10. Possible hydrogen bonds

Donor	H	Acceptor	D...A	D-H	H...A	D-H...A
O1	H1	O3[1]	2.786(4)	0.84	2.04	148.18
O2	H2	O2[2]	3.030(4)	0.84	2.55	117.14

Symmetry Operators:

(1) -X+1,Y,-Z+1/2+1

(2) -X+1/2,-Y+1/2+2,-Z+1

Table 11. Intramolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Br1	O1	3.244(3)	Br1	C8	3.278(4)
Br1	B1	3.481(4)	Br2	C4	3.316(4)
Br2	C12	3.348(3)	Br2	C13	3.552(3)
Br2	B1	3.433(4)	Br3	O1	3.475(3)
Br3	C18	3.282(4)	Br3	B1	3.472(4)
Br4	C2	3.447(4)	Br4	C14	3.320(4)
Br4	B1	3.440(4)	Br5	C28	3.302(4)
Br5	C32	3.455(4)	Br5	B2	3.432(4)
Br6	O2	3.457(4)	Br6	C24	3.282(4)
Br6	B2	3.465(4)	Br7	C22	3.343(3)
Br7	C38	3.308(4)	Br7	B2	3.413(4)
Br8	O2	3.424(4)	Br8	C34	3.282(4)
Br8	B2	3.510(4)	O1	C1	3.095(4)
O1	C11	3.286(5)	O2	C23	3.273(5)
O2	C33	3.197(5)	O5	C45	3.563(13)
C2	C13	3.396(5)	C3	C12	3.363(5)
C4	C7	3.142(6)	C4	C8	3.177(5)
C5	C8	3.153(6)	C5	C9	3.161(5)
C6	C9	3.124(5)	C6	C10	3.133(6)
C7	C10	3.169(6)	C14	C17	3.150(5)
C14	C18	3.168(5)	C15	C18	3.144(5)
C15	C19	3.159(6)	C16	C19	3.131(6)
C16	C20	3.142(6)	C17	C20	3.177(5)
C21	C32	3.376(5)	C22	C31	3.339(5)
C24	C27	3.130(5)	C24	C28	3.166(5)
C25	C28	3.153(6)	C25	C29	3.166(6)
C26	C29	3.128(6)	C26	C30	3.129(5)
C27	C30	3.155(5)	C34	C37	3.144(5)
C34	C38	3.171(5)	C35	C38	3.155(6)
C35	C39	3.165(6)	C36	C39	3.123(6)
C36	C40	3.124(5)	C37	C40	3.162(5)
C42	C45	3.567(18)			

Table 12. Intramolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Br1	H8	2.831	Br2	H4	2.875
Br3	H1	3.013	Br3	H18	2.830
Br4	H14	2.879	Br5	H28	2.863
Br6	H2	3.562	Br6	H24	2.832
Br7	H38	2.865	Br8	H34	2.828
C1	H8	2.656	C2	H1	3.186
C3	H4	2.656	C4	H6	3.291
C5	H7	3.299	C6	H4	3.292
C6	H8	3.306	C7	H5	3.302
C8	H6	3.299	C9	H4	3.383
C9	H7	3.290	C10	H5	3.300
C10	H8	3.398	C11	H1	2.966
C11	H18	2.644	C12	H1	2.535
C13	H14	2.658	C14	H16	3.300
C15	H17	3.308	C16	H14	3.302
C16	H18	3.301	C17	H15	3.305
C18	H16	3.300	C19	H14	3.381
C19	H17	3.298	C20	H15	3.298
C20	H18	3.386	C21	H28	2.650
C22	H2	2.635	C23	H2	3.292
C23	H24	2.641	C24	H26	3.290
C25	H27	3.294	C26	H24	3.289
C26	H28	3.308	C27	H25	3.298
C28	H26	3.305	C29	H24	3.379
C29	H27	3.286	C30	H25	3.302
C30	H28	3.380	C31	H38	2.653
C32	H2	3.108	C33	H34	2.641
C34	H36	3.288	C35	H37	3.307
C36	H34	3.291	C36	H38	3.304
C37	H35	3.309	C38	H36	3.297
C39	H34	3.379	C39	H37	3.296
C40	H35	3.299	C40	H38	3.383
H4	H5	2.207	H5	H6	2.197
H6	H7	2.200	H7	H8	2.213
H14	H15	2.205	H15	H16	2.206
H16	H17	2.206	H17	H18	2.214
H24	H25	2.208	H25	H26	2.201

Table 12. Intramolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H26	H27	2.197	H27	H28	2.216
H34	H35	2.208	H35	H36	2.201
H36	H37	2.201	H37	H38	2.216

Table 13. Intermolecular contacts less than 3.60 Å

atom	atom	distance	atom	atom	distance
Br3	O3[1]	3.568(3)	Br4	C24	3.541(4)
Br5	C18[2]	3.316(4)	Br5	C19[2]	3.366(3)
Br6	O2[3]	3.481(3)	Br6	C34[4]	3.540(4)
Br6	C35[4]	3.537(4)	Br6	C38[5]	3.531(4)
O1	O3[1]	2.786(4)	O1	C42[1]	3.428(13)
O1	C44	3.514(6)	O1	C44[1]	3.391(6)
O1	C46	3.595(10)	O2	Br6[3]	3.481(3)
O2	O2[3]	3.030(4)	O3	Br3[1]	3.568(3)
O3	O1[1]	2.786(4)	O3	C26[6]	3.464(5)
O4	C9	3.575(9)	C2	C44	3.575(6)
C2	C46	3.591(9)	C6	C45	3.474(14)
C7	C45	3.554(14)	C8	C25	3.563(6)
C8	C26	3.576(6)	C8	C43	3.521(7)
C9	O4	3.575(9)	C9	C25	3.523(5)
C11	C26[7]	3.403(5)	C14	C24[7]	3.497(5)
C16	C23[7]	3.428(5)	C16	C30[7]	3.515(5)
C16	C34[8]	3.594(6)	C17	C29[7]	3.398(5)
C17	C30[7]	3.574(5)	C18	Br5[8]	3.316(4)
C18	C28[7]	3.460(5)	C18	C29[7]	3.545(5)
C19	Br5[8]	3.366(3)	C19	C25[7]	3.528(5)
C19	C26[7]	3.482(5)	C20	C24[7]	3.495(5)
C20	C25[7]	3.419(5)	C23	C16[5]	3.428(5)
C24	Br4	3.541(4)	C24	C14[5]	3.497(5)
C24	C20[5]	3.495(5)	C25	C8	3.563(6)
C25	C9	3.523(5)	C25	C19[5]	3.528(5)
C25	C20[5]	3.419(5)	C26	O3[6]	3.464(5)
C26	C8	3.576(6)	C26	C11[5]	3.403(5)
C26	C19[5]	3.482(5)	C28	C18[5]	3.460(5)
C29	C17[5]	3.398(5)	C29	C18[5]	3.545(5)
C30	C16[5]	3.515(5)	C30	C17[5]	3.574(5)
C34	Br6[9]	3.540(4)	C34	C16[2]	3.594(6)
C35	Br6[9]	3.537(4)	C38	Br6[7]	3.531(4)
C42	O1[1]	3.428(13)	C43	C8	3.521(7)
C43	C45[10]	3.537(14)	C44	O1	3.514(6)
C44	O1[1]	3.391(6)	C44	C2	3.575(6)
C45	C6	3.474(14)	C45	C7	3.554(14)
C45	C43[10]	3.537(14)	C45	C45[10]	2.59(2)

Table 13. Intermolecular contacts less than 3.60 Å (continued)

atom	atom	distance	atom	atom	distance
C46	O1	3.595(10)	C46	C2	3.591(9)

Symmetry Operators:

(1) -X+1,Y,-Z+1/2+1
(2) X,Y+1,Z
(3) -X+1/2,-Y+1/2+2,-Z+1
(4) -X+1/2,Y+1/2-1,-Z+1/2+1
(5) X,-Y+2,Z+1/2-1
(6) -X+1,-Y+2,-Z+1
(7) X,-Y+2,Z+1/2
(8) X,Y-1,Z
(9) -X+1/2,Y+1/2,-Z+1/2+1
(10) -X+1,Y,-Z+1/2

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens

atom	atom	distance	atom	atom	distance
Br1	H6[1]	3.311	Br1	H7[2]	3.222
Br1	H7[1]	3.069	Br1	H8[2]	3.499
Br2	H17[3]	3.400	Br2	H18[3]	3.008
Br2	H28[4]	3.189	Br2	H37[5]	3.582
Br3	H4[6]	3.572	Br4	H6[1]	3.257
Br4	H24	3.595	Br4	H37[5]	3.045
Br5	H5[1]	3.467	Br5	H18[7]	3.518
Br5	H36[8]	3.572	Br6	H2[9]	3.070
Br6	H15[5]	3.593	Br6	H34[10]	2.886
Br6	H35[10]	2.891	Br6	H38[5]	3.168
Br7	H4[1]	3.569	Br7	H5[1]	3.446
Br7	H14	3.186	Br7	H24[1]	3.238
Br8	H15[11]	2.995	Br8	H35[8]	3.039
Br8	H36[8]	3.427	O1	H7[1]	2.805
O2	H2[9]	2.553	O2	H15[11]	2.954
O2	H16[11]	3.081	O2	H34[10]	3.590
O2	H35[8]	3.168	O3	H1[12]	2.036
O3	H7[2]	3.528	O3	H8[2]	3.007
O3	H26[2]	2.613	O3	H27[2]	3.325
O5	H1[12]	3.595	C4	H25	3.470
C5	H25	3.578	C6	H25	3.441
C7	H1[5]	3.554	C7	H25	3.143
C7	H26	3.476	C8	H25	2.911
C8	H26	2.933	C9	H25	2.920
C9	H26	3.447	C10	H25	3.188
C11	H26[1]	3.395	C12	H26[1]	3.584
C13	H25[1]	3.400	C13	H37[5]	3.242
C14	H24[1]	3.361	C14	H36[5]	3.156
C14	H37[5]	2.876	C15	H36[5]	3.114
C16	H34[4]	3.530	C20	H25[1]	3.526
C20	H37[5]	3.167	C21	H5[1]	3.185
C21	H17[5]	3.428	C22	H16[5]	3.505
C23	H16[5]	3.460	C26	H8	3.473
C27	H5[1]	3.567	C27	H6[1]	3.456
C27	H18[5]	3.495	C28	H5[1]	2.843
C28	H6[1]	3.589	C28	H18[5]	3.325
C29	H5[1]	2.945	C29	H17[5]	3.489

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
C33	H15[11]	3.256	C33	H16[7]	3.585
C34	H16[7]	2.860	C34	H17[7]	3.232
C35	H2[13]	3.313	C35	H16[7]	3.455
C35	H17[7]	3.468	C37	H14[1]	3.371
C38	H17[7]	3.545	C39	H17[7]	3.304
C40	H16[7]	3.257	C40	H17[7]	3.143
C41	H1[12]	3.159	C41	H26[2]	3.458
C41	H27[2]	3.500	C42	H1[12]	2.784
C43	H27[2]	3.328	C44	H1[12]	3.072
C46	H27[4]	3.106	B1	H7[1]	3.182
B2	H35[8]	3.508	H1	O3[12]	2.036
H1	O5[12]	3.595	H1	C7[1]	3.554
H1	C41[12]	3.159	H1	C42[12]	2.784
H1	C44[12]	3.072	H1	H7[1]	2.832
H1	H26[1]	3.168	H2	Br6[9]	3.070
H2	O2[9]	2.553	H2	C35[8]	3.313
H2	H2[9]	2.295	H2	H15[11]	3.470
H2	H16[5]	3.073	H2	H16[11]	3.546
H2	H34[8]	3.287	H2	H35[8]	2.645
H4	Br3[3]	3.572	H4	Br7[5]	3.569
H4	H18[3]	2.843	H5	Br5[5]	3.467
H5	Br7[5]	3.446	H5	C21[5]	3.185
H5	C27[5]	3.567	H5	C28[5]	2.843
H5	C29[5]	2.945	H5	H28[5]	2.812
H6	Br1[5]	3.311	H6	Br4[5]	3.257
H6	C27[5]	3.456	H6	C28[5]	3.589
H7	Br1[2]	3.222	H7	Br1[5]	3.069
H7	O1[5]	2.805	H7	O3[2]	3.528
H7	B1[5]	3.182	H7	H1[5]	2.832
H7	H26	3.559	H8	Br1[2]	3.499
H8	O3[2]	3.007	H8	C26	3.473
H8	H8[2]	3.198	H8	H25	3.355
H8	H26	2.689	H14	Br7	3.186
H14	C37[5]	3.371	H14	H24[1]	3.473
H14	H36[5]	3.241	H14	H37[5]	2.539
H15	Br6[1]	3.593	H15	Br8[10]	2.995
H15	O2[10]	2.954	H15	C33[10]	3.256

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H15	H2[10]	3.470	H15	H36[5]	3.143
H16	O2[10]	3.081	H16	C22[1]	3.505
H16	C23[1]	3.460	H16	C33[4]	3.585
H16	C34[4]	2.860	H16	C35[4]	3.455
H16	C40[4]	3.257	H16	H2[1]	3.073
H16	H2[10]	3.546	H16	H34[4]	2.685
H17	Br2[6]	3.400	H17	C21[1]	3.428
H17	C29[1]	3.489	H17	C34[4]	3.232
H17	C35[4]	3.468	H17	C38[4]	3.545
H17	C39[4]	3.304	H17	C40[4]	3.143
H18	Br2[6]	3.008	H18	Br5[4]	3.518
H18	C27[1]	3.495	H18	C28[1]	3.325
H18	H4[6]	2.843	H18	H28[1]	3.455
H24	Br4	3.595	H24	Br7[5]	3.238
H24	C14[5]	3.361	H24	H14[5]	3.473
H24	H38[5]	2.802	H25	C4	3.470
H25	C5	3.578	H25	C6	3.441
H25	C7	3.143	H25	C8	2.911
H25	C9	2.920	H25	C10	3.188
H25	C13[5]	3.400	H25	C20[5]	3.526
H25	H8	3.355	H26	O3[2]	2.613
H26	C7	3.476	H26	C8	2.933
H26	C9	3.447	H26	C11[5]	3.395
H26	C12[5]	3.584	H26	C41[2]	3.458
H26	H1[5]	3.168	H26	H7	3.559
H26	H8	2.689	H27	O3[2]	3.325
H27	C41[2]	3.500	H27	C43[2]	3.328
H27	C46[7]	3.106	H28	Br2[7]	3.189
H28	H5[1]	2.812	H28	H18[5]	3.455
H34	Br6[11]	2.886	H34	O2[11]	3.590
H34	C16[7]	3.530	H34	H2[13]	3.287
H34	H16[7]	2.685	H35	Br6[11]	2.891
H35	Br8[13]	3.039	H35	O2[13]	3.168
H35	B2[13]	3.508	H35	H2[13]	2.645
H36	Br5[13]	3.572	H36	Br8[13]	3.427
H36	C14[1]	3.156	H36	C15[1]	3.114
H36	H14[1]	3.241	H36	H15[1]	3.143

Table 14. Intermolecular contacts less than 3.60 Å involving hydrogens (continued)

atom	atom	distance	atom	atom	distance
H37	$Br2^{1}$	3.582	H37	$Br4^{1}$	3.045
H37	$C13^{1}$	3.242	H37	$C14^{1}$	2.876
H37	$C20^{1}$	3.167	H37	$H14^{1}$	2.539
H38	$Br6^{1}$	3.168	H38	$H24^{1}$	2.802

Symmetry Operators:

(1) X,-Y+2,Z+1/2
(2) -X+1,-Y+2,-Z+1
(3) X,-Y+1,Z+1/2-1
(4) X,Y-1,Z
(5) X,-Y+2,Z+1/2-1
(6) X,-Y+1,Z+1/2
(7) X,Y+1,Z
(8) X,-Y+3,Z+1/2-1
(9) -X+1/2,-Y+1/2+2,-Z+1
(10) -X+1/2,Y+1/2-1,-Z+1/2+1
(11) -X+1/2,Y+1/2,-Z+1/2+1
(12) -X+1,Y,-Z+1/2+1
(13) X,-Y+3,Z+1/2