

Electronic Supplementary Information (ESI)

Synthesis of Carborane-Fused Carbo- and Heterocycles via Zirconacyclopentane Intermediate

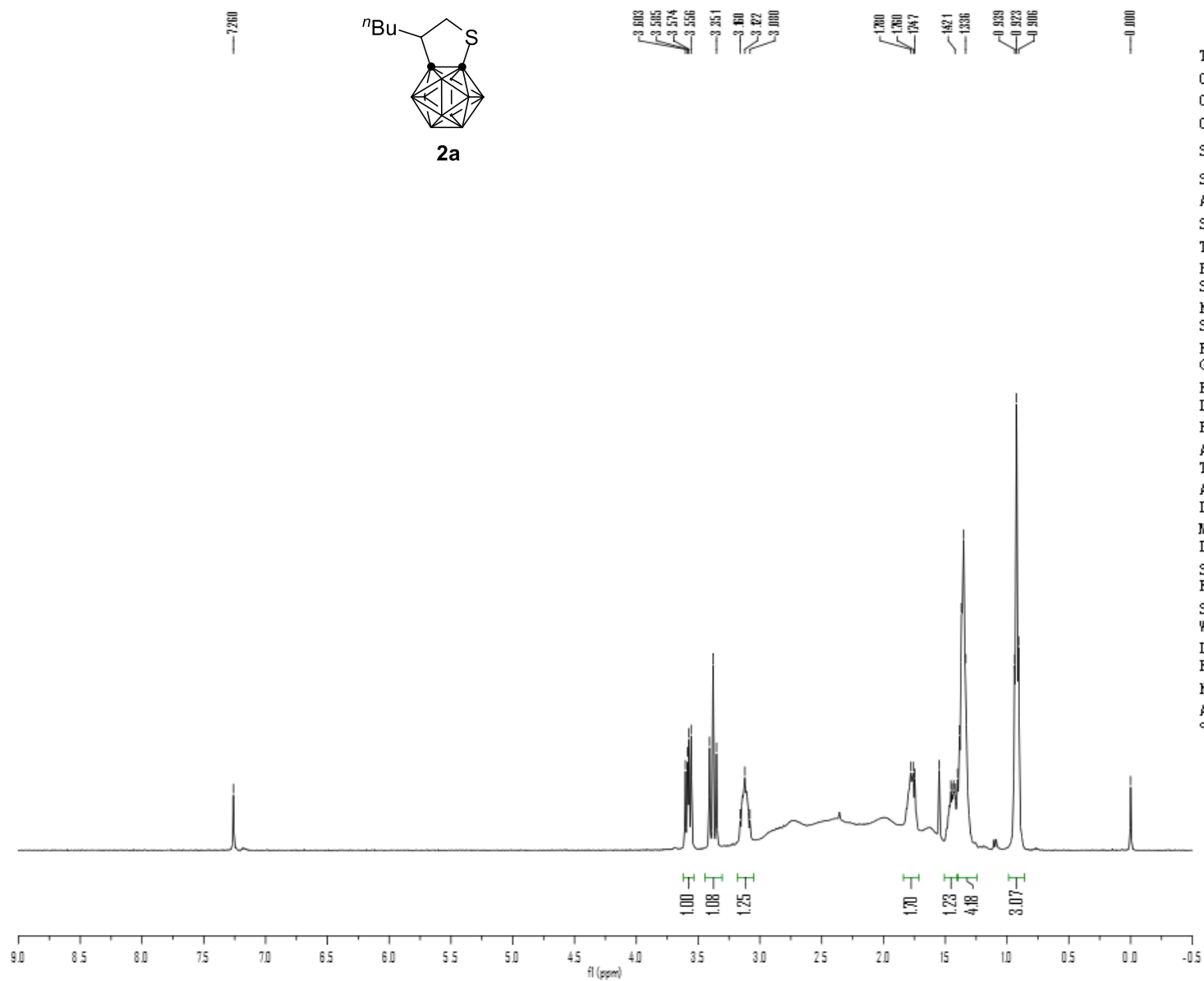
Chun-Xiao Cui, Shikuo Ren, Zaozao Qiu* and Zuowei Xie*

Table of Contents

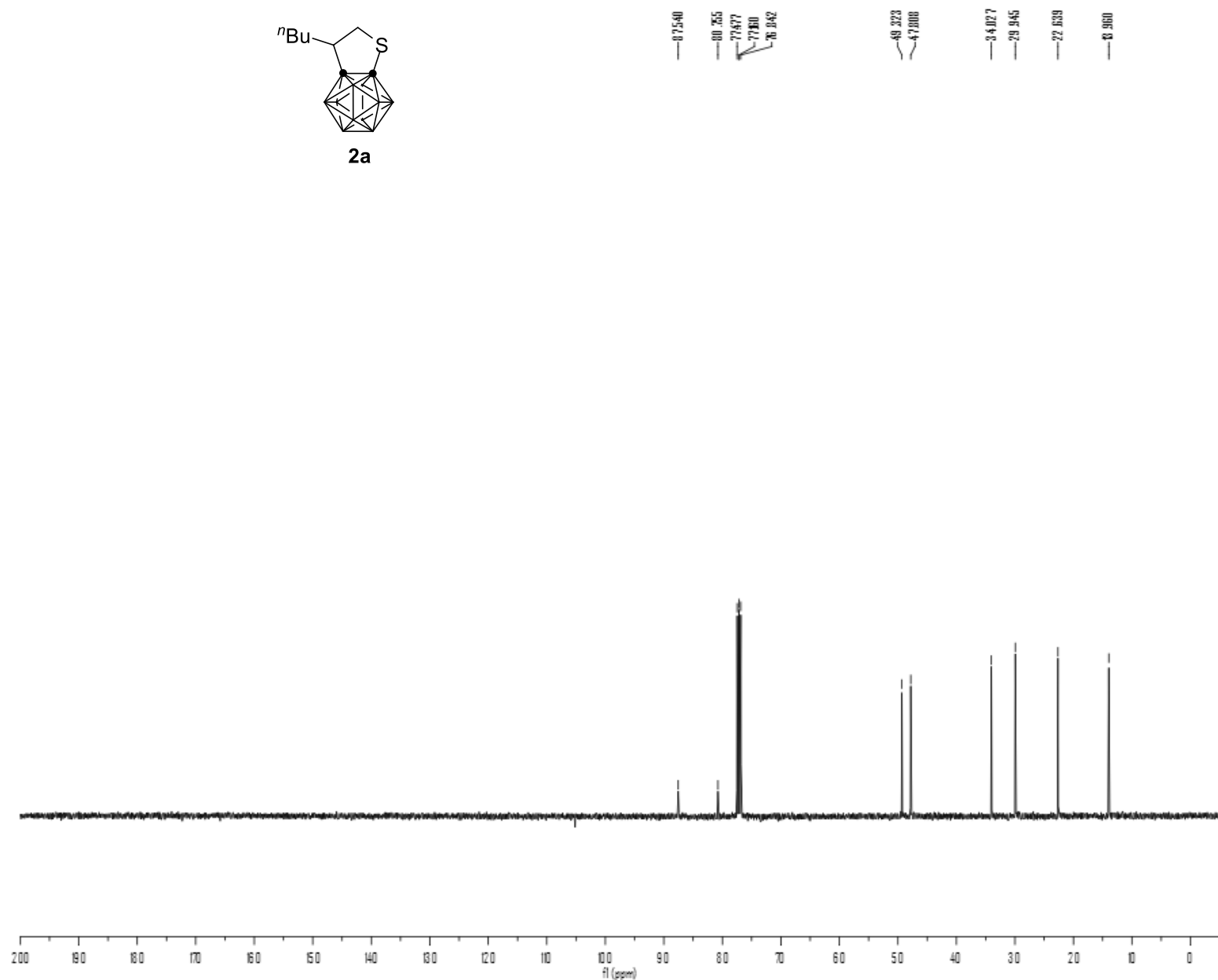
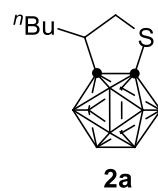
1. Crystal Data and Summary of Data Collection and Refinements	S2
2. NMR Spectra	S3

Table S1. Crystal Data and Summary of Data Collection and Refinement for **2c**, **6**, **7** and **11**.

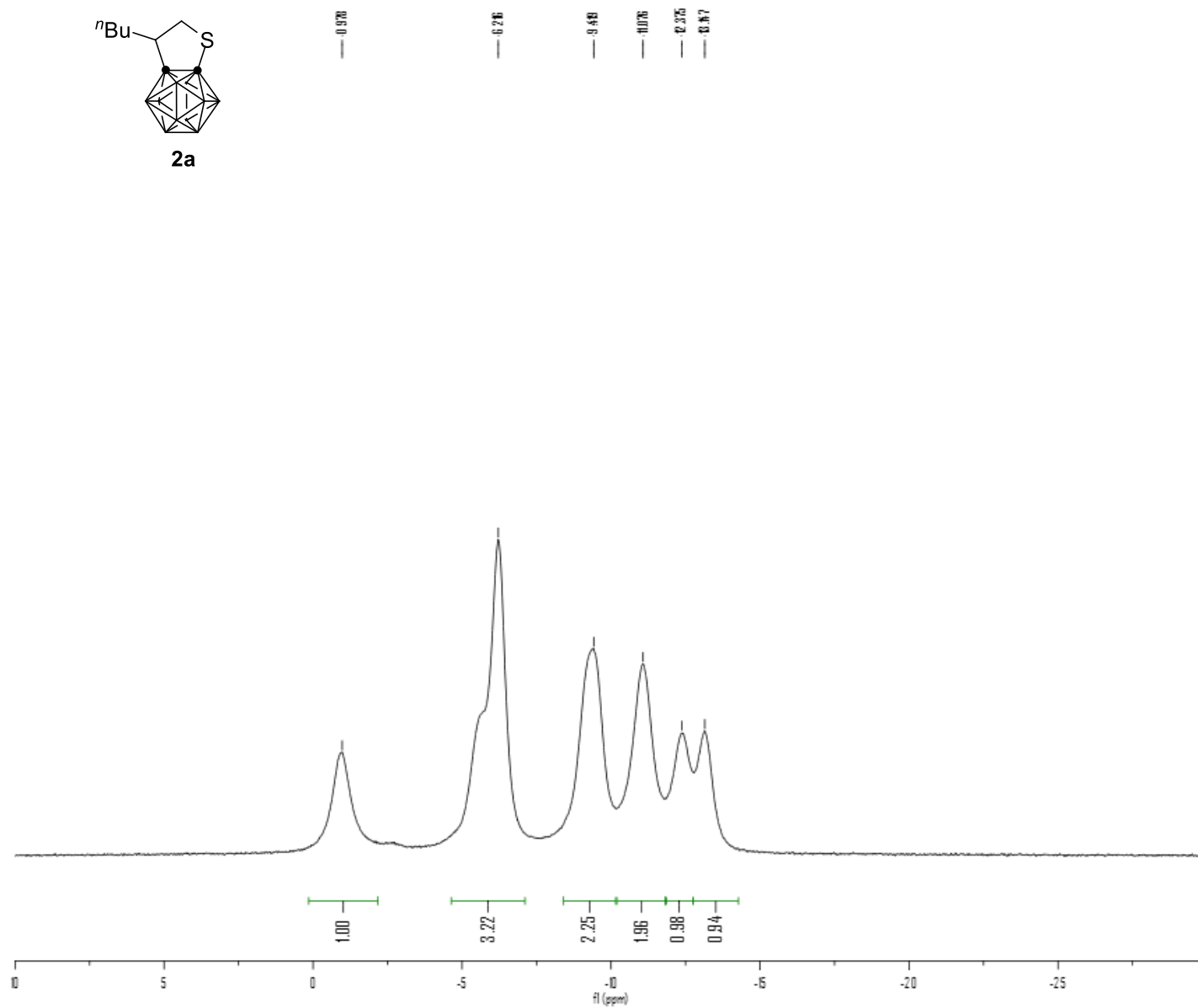
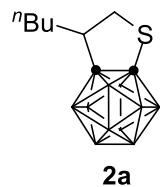
compound	2c	6	7	11
formula	C ₈ H ₂₂ B ₁₀ Te	C ₉ H ₂₂ B ₁₀ O	C ₂₁ H ₃₆ B ₁₀ N ₂ O ₂ Zr	C ₁₄ H ₂₇ B ₁₀ OP
crystal size (mm)	0.12 x 0.08 x 0.05	0.35 x 0.30 x 0.18	0.2 x 0.1 x 0.01	0.40 x 0.30 x 0.20
fw	353.95	254.36	547.84	350.43
crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic
space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> (-1)	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> Å	14.833(1)	9.737(0)	9.711(2)	14.078(1)
<i>b</i> Å	9.687(1)	6.795(1)	10.502(2)	9.460(1)
<i>c</i> Å	23.421(1)	22.715(3)	13.566(3)	15.4850(7)
<i>α</i> , deg	90	90	79.777(4)	90
<i>β</i> , deg	107.598(1)	98.023(2)	72.418(3)	92.295(1)
<i>γ</i> , deg	90	90	88.988(3)	90
<i>V</i> , Å ³	3207.8(2)	1488.3(3)	1297.0(4)	2060.6(2)
<i>Z</i>	8	4	2	4
<i>D</i> _{calcd} , Mg/m ³	1.466	1.135	1.403	1.130
radiation (λ) Å	1.34139	0.71073	0.71073	0.71073
2θ range, deg	9.7 to 121.4	3.6 to 61.1	3.9 to 61.5	3.8 to 50.5
μ, mm ⁻¹	9.747	0.058	0.448	0.133
<i>F</i> (000)	1376	536	564	736
no. of params refnd	345	182	327	235
no. of obsd reflns	7309	4555	7937	3734
goodness of fit	1.080	1.083	0.851	1.042
R1	0.066	0.060	0.050	0.048
wR2	0.182	0.157	0.124	0.124



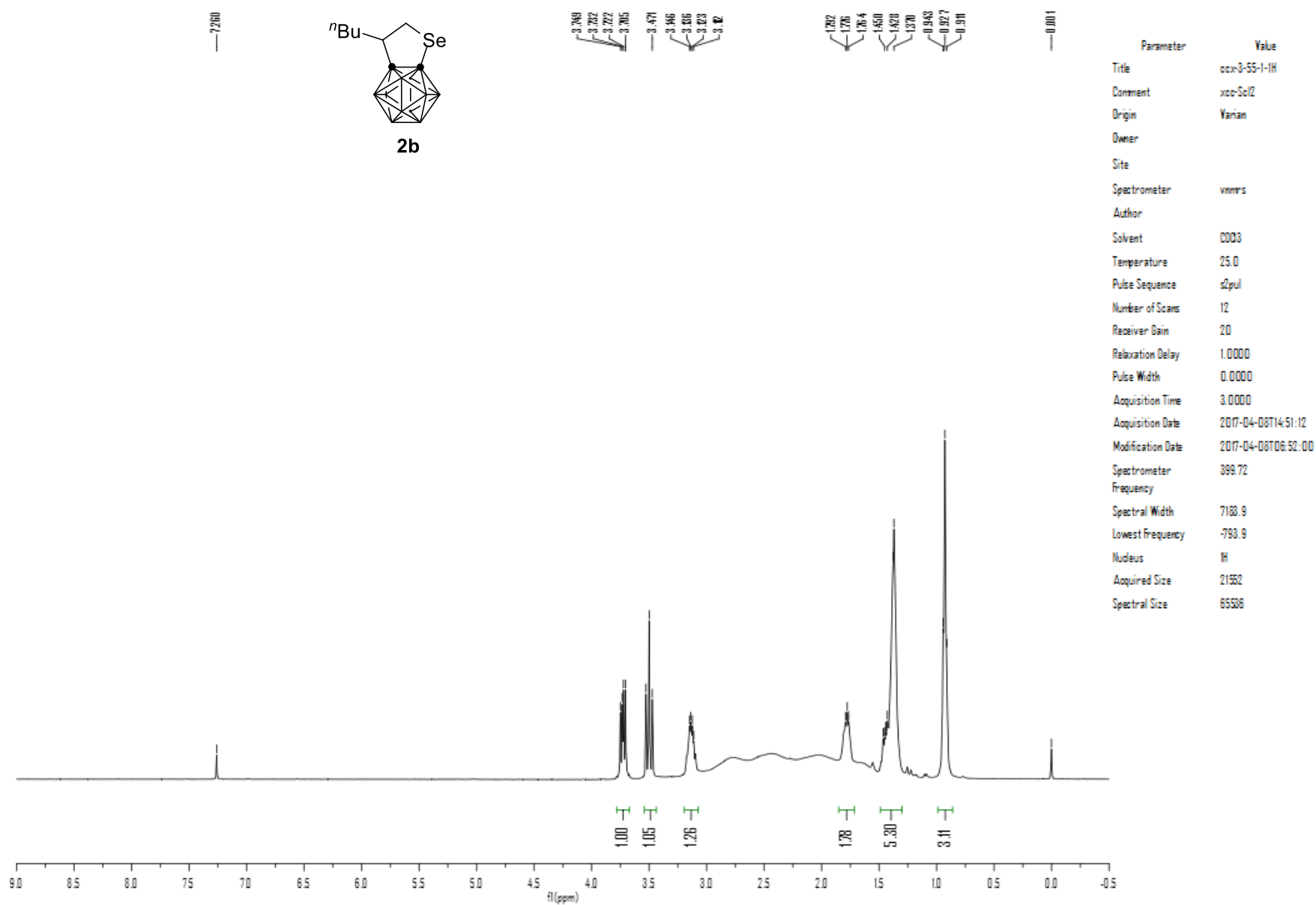
Parameter	Value
Title	cox-7-90-1H
Comment	Std proton
Origin	Varian
Owner	
Site	
Spectrometer	vmrs
Author	omc1
Solvent	CDCl ₃
Temperature	20.0
Pulse	s2pul
Sequence	
Number of Scans	12
Receiver	30
Gain	
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-04-14T23:00
Modification Date	2017-04-14T15:01
Spectrometer Frequency	400.03
Spectral Width	7267.4
Lowest Frequency	-645.9
Nucleus	¹ H
Acquired	21802
Size	

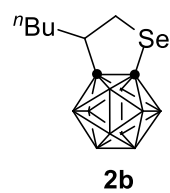


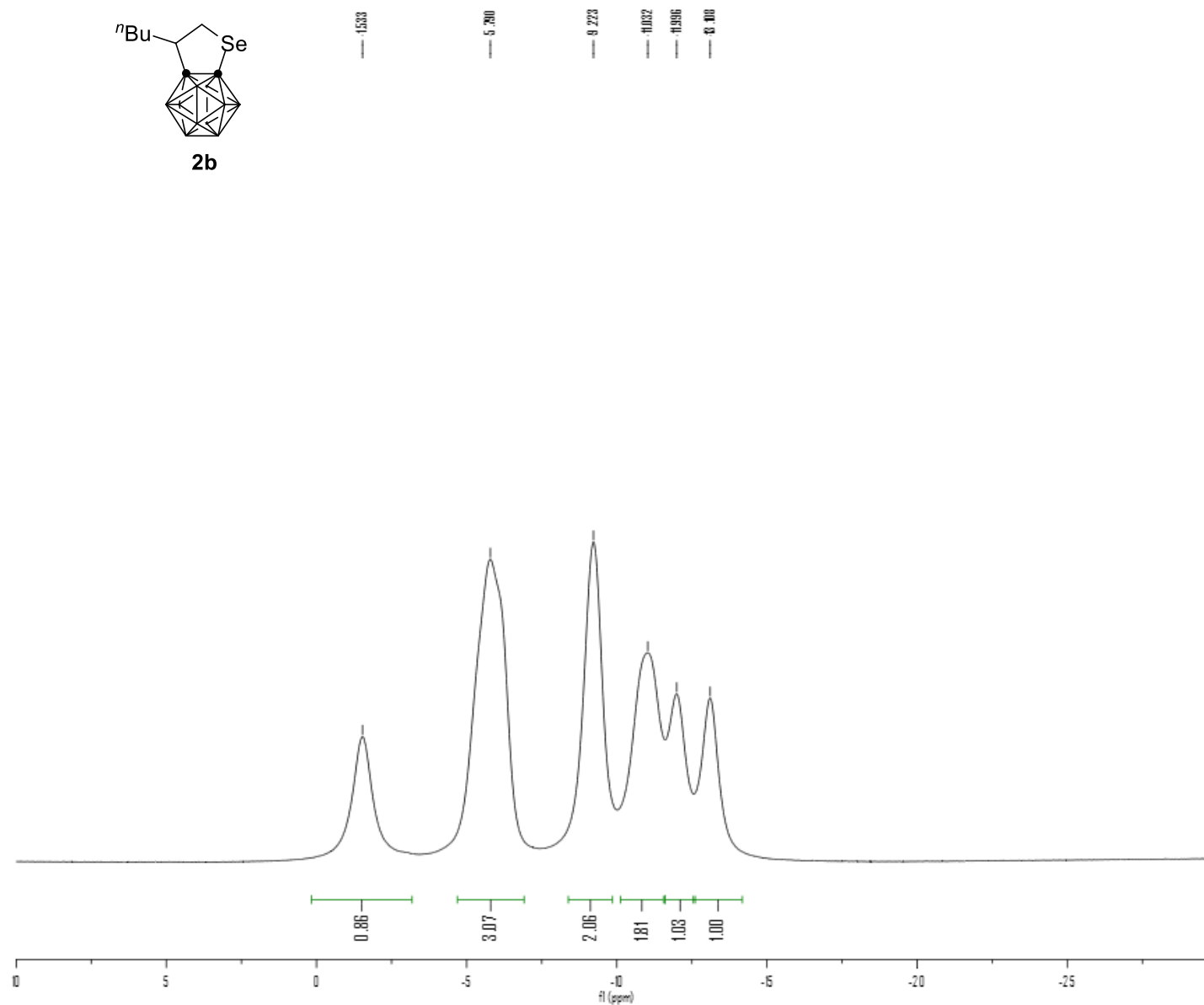
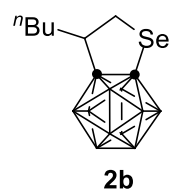
Parameter	Value
Title	ccc-7-90-1-C-0
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	omc1
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	sQpul
Number of Scans	480
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-04-14T23:10:25
Modification Date	2017-04-14T15:29:00
Spectrometer	100.60
Frequency	
Spectral Width	24509.8
Lowest Frequency	-1676.8
Nucleus	13C
Acquired Size	31875
Spectral Size	65536



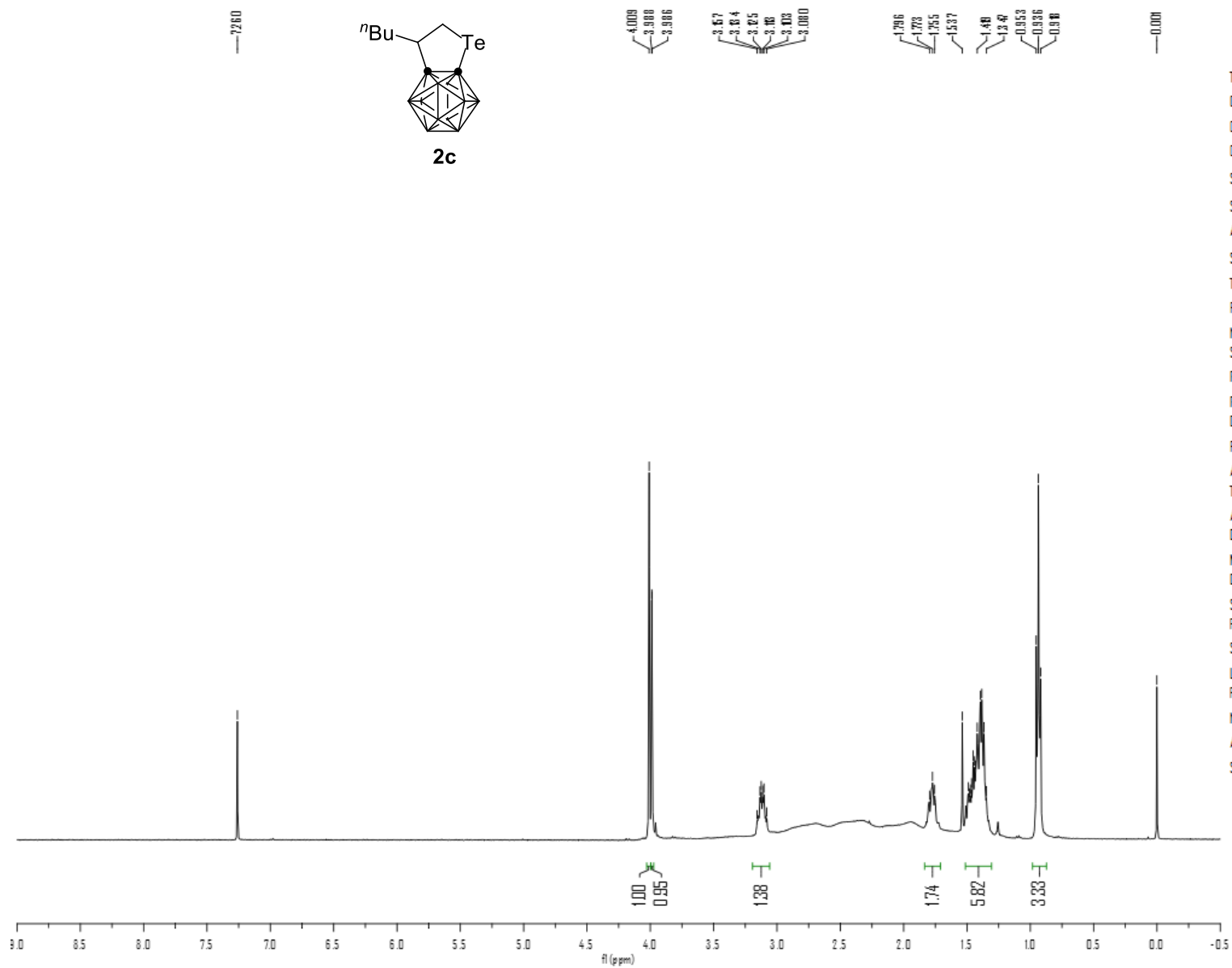
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-coc-7-90-1/1/pdata/1/1r
Title	20120606-coc-7-90-1
Comment	
Origin	UXMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	dmx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	zing_1gy
Number of Scans	50
Receiver Gain	203
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-04-17T22:32:07
Modification Date	2017-04-17T16:05:46
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16379.7
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



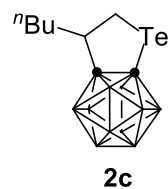


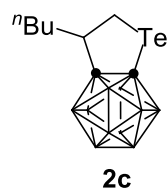


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/b-cxx-3-55-1/pdata/1/1r
Title	Desktop
Comment	
Origin	WQMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.fgy
Number of Scans	800
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.3185
Acquisition Date	2015-04-16T22:07:43
Modification Date	2015-04-16T16:07:00
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-17920.9
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

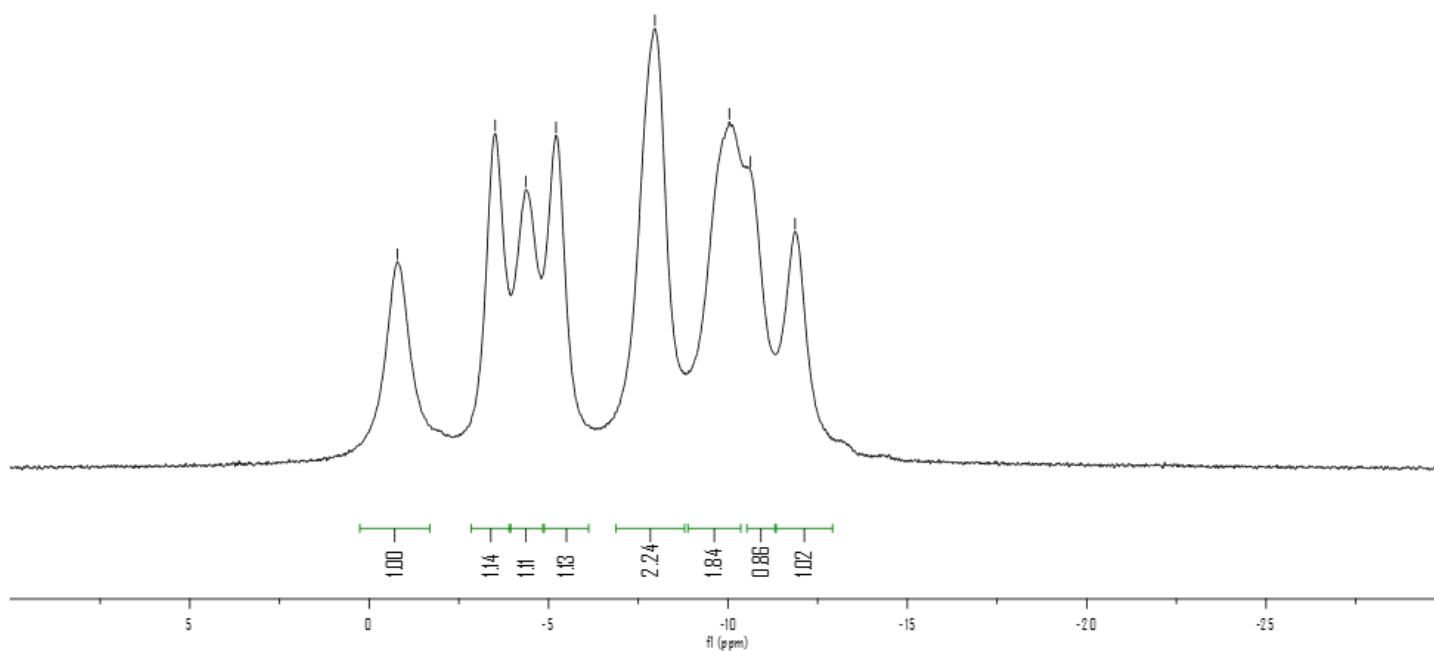


Parameter	Value
Title	ccx-8-18-1
Comment	xc-c-Sc12
Origin	Varian
Owner	
Site	
Spectrometer	vnmr5
Author	
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	32
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-05-17T12:21:11
Modification Date	2017-05-17T04:22:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-783.5
Nucleus	¹ H
Acquired Size	21552
Spectral Size	65536

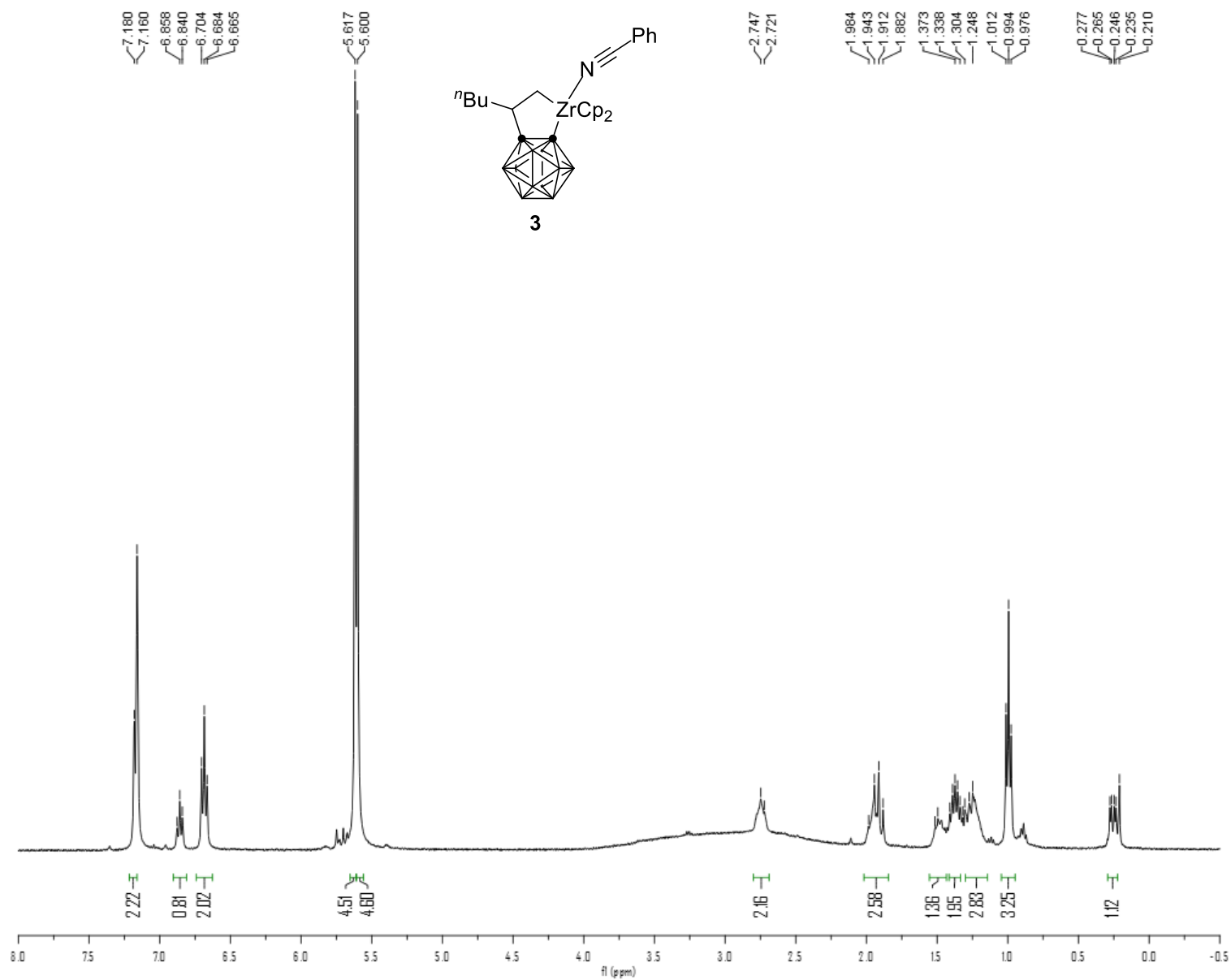




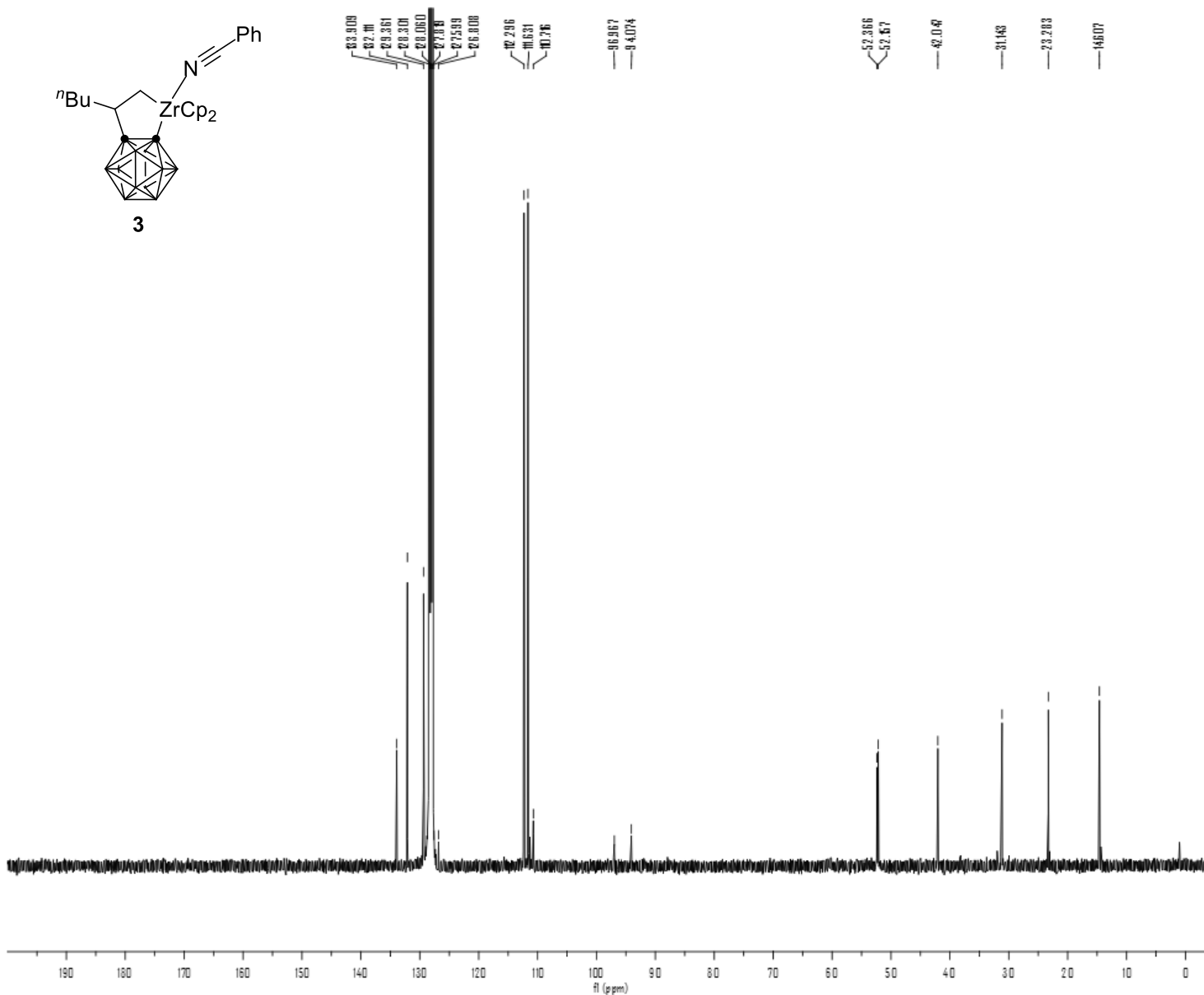
0.708
3.50
4.364
5.208
7.664
10.039
10.627
11.872

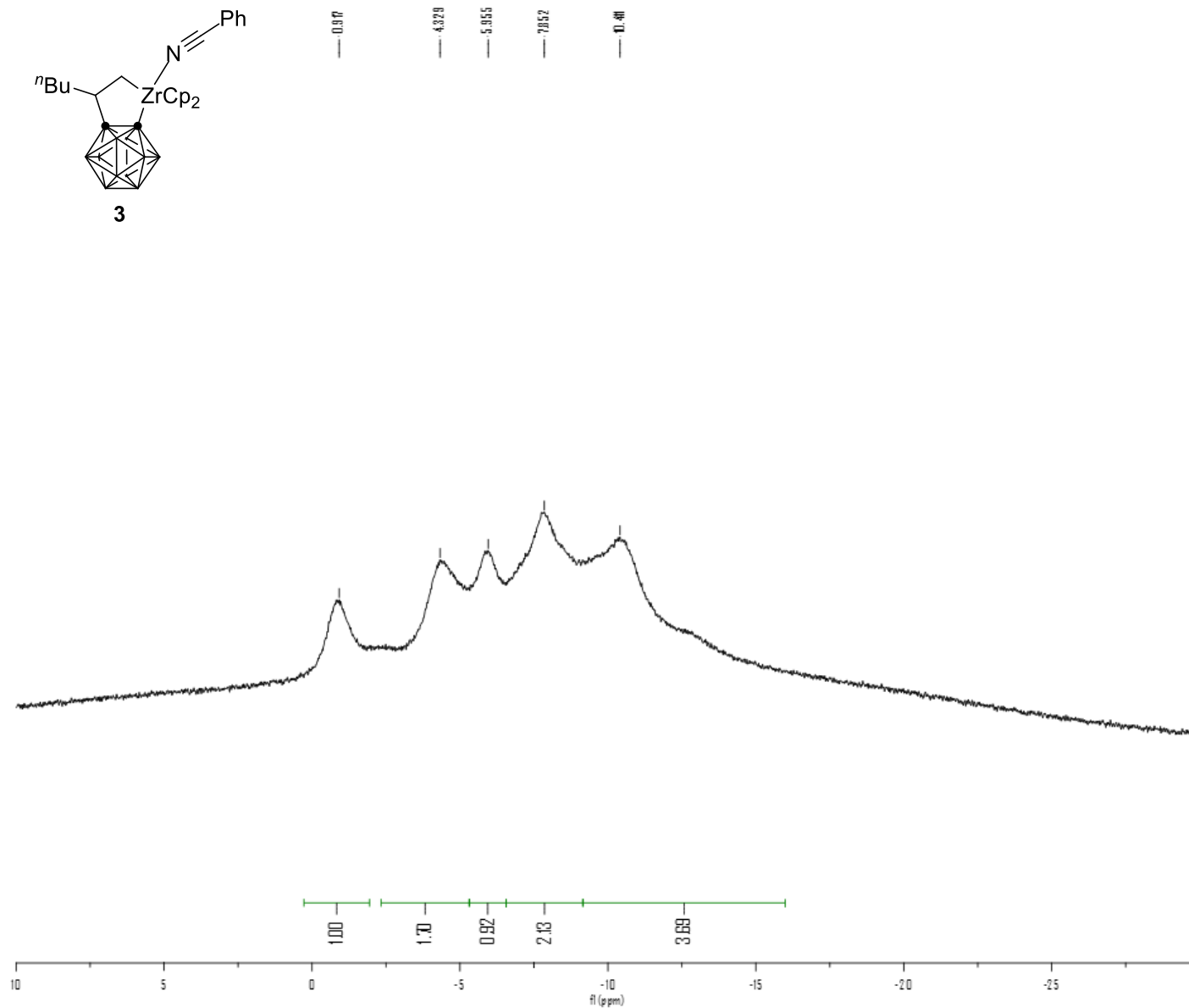
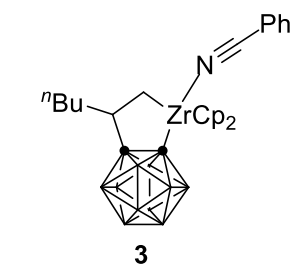


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-ccx-8-18-1/pdata/1/1r
Title	20120606-ccx-8-18-1
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring1gy
Number of Scans	123
Receiver Gain	406
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.3195
Acquisition Date	2017-05-18T19:02:57
Modification Date	2017-05-18T13:17:50
Spectrometer	128.38
Frequency	
Spectral Width	51282.1
Lowest Frequency	-25883.4
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

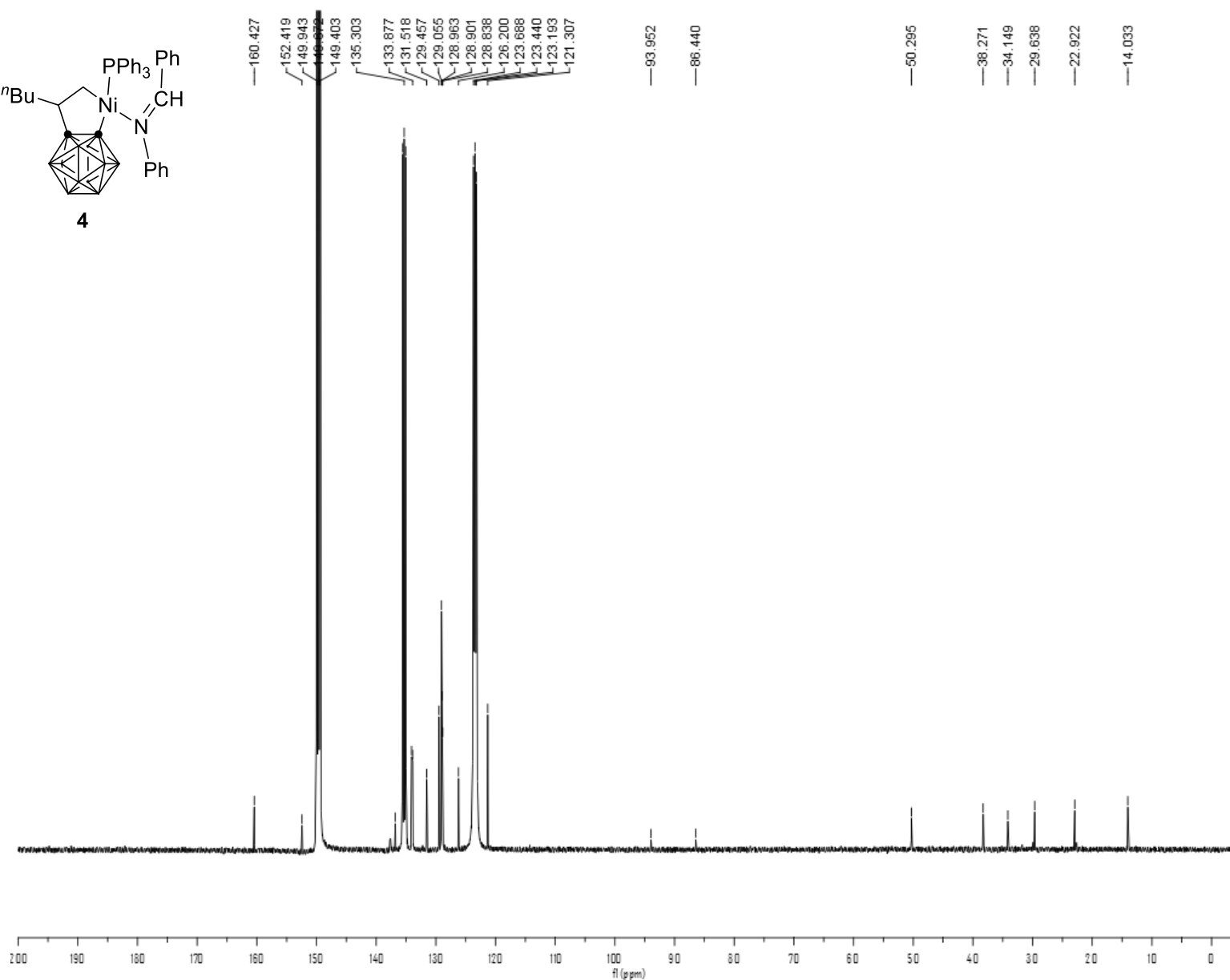
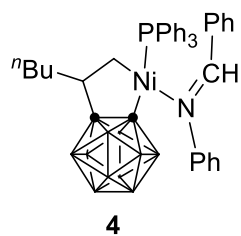


Parameter	Value
Title	ccx-7-88-2
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	32
Receiver Gain	6
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	2.2807
Acquisition Date	2017-05-10T00:26:05
Modification Date	2017-05-09T16:28:00
Spectrometer Frequency	399.72
Spectral Width	7183.9
Lowest Frequency	-777.4
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

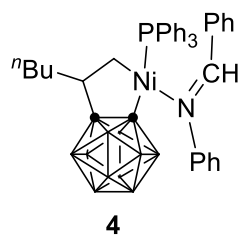
S13



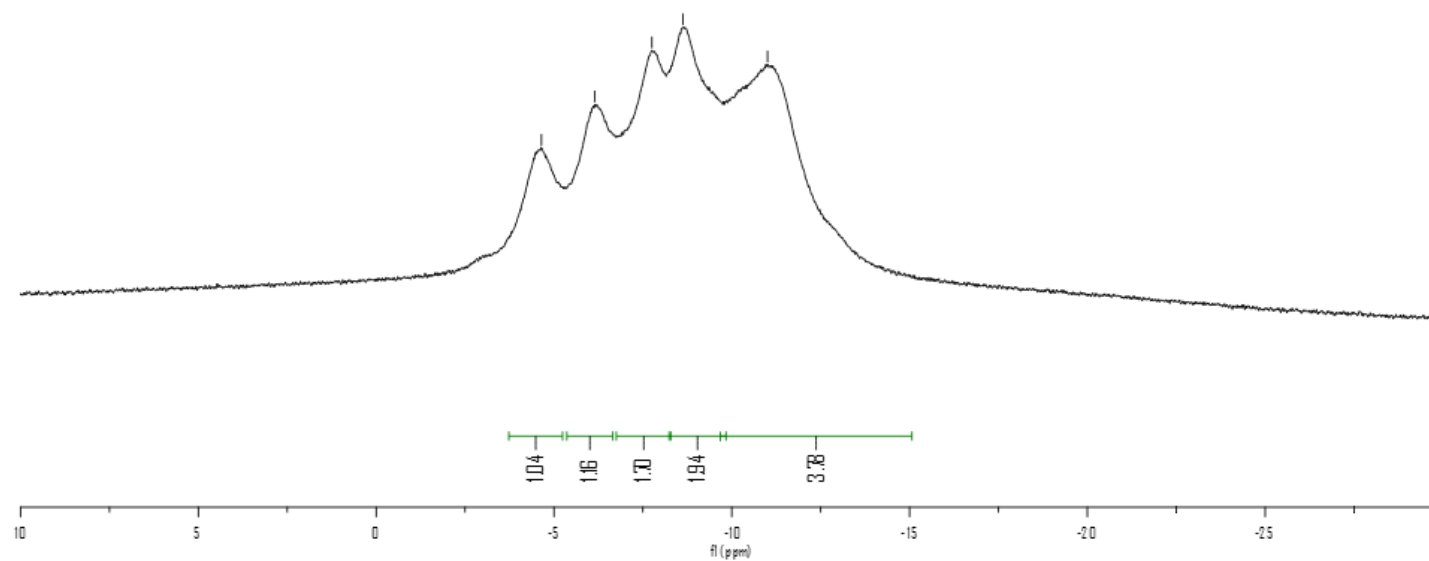
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-cx-x-7-88-1/1/pdata/1/1r
Title	20120606-cx-x-7-88-1
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	300.0
Pulse Sequence	zgpg30
Number of Scans	10.00
Receiver Gain	362
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-04-17T22:37:55
Modification Date	2017-04-17T16:05:38
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16379.7
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



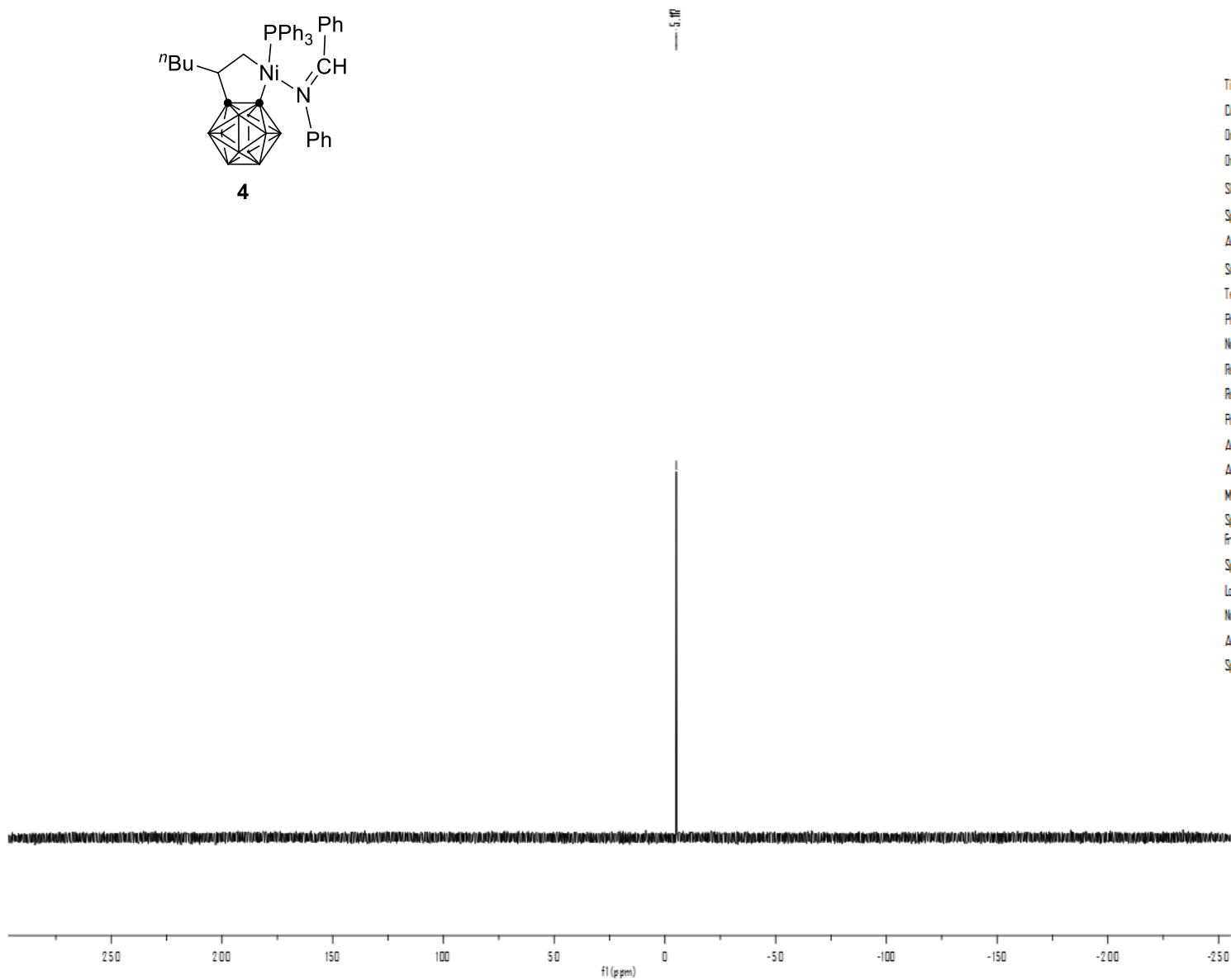
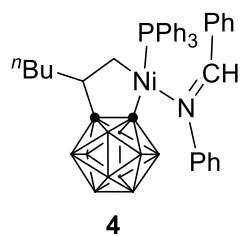
Parameter	Value
Title	ccx-7-10-3-3-ccc
Comment	new experiment
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	pyridine
Temperature	25.0
Pulse Sequence	s2pul
Number of	5844
Scans	
Receiver Gain	60
Relaxation	1.0000
Delay	
Pulse Width	0.0000
Acquisition	1.7826
Time	
Acquisition	2017-06-23T02:07:43
Date	
Modification	2017-06-22T22:44:00
Date	
Spectrometer	100.53
Frequency	
Spectral Width	36764.7
Lowest	-856.4
Frequency	
Nucleus	13C
Acquired Size	65536
Spectral Size	131072



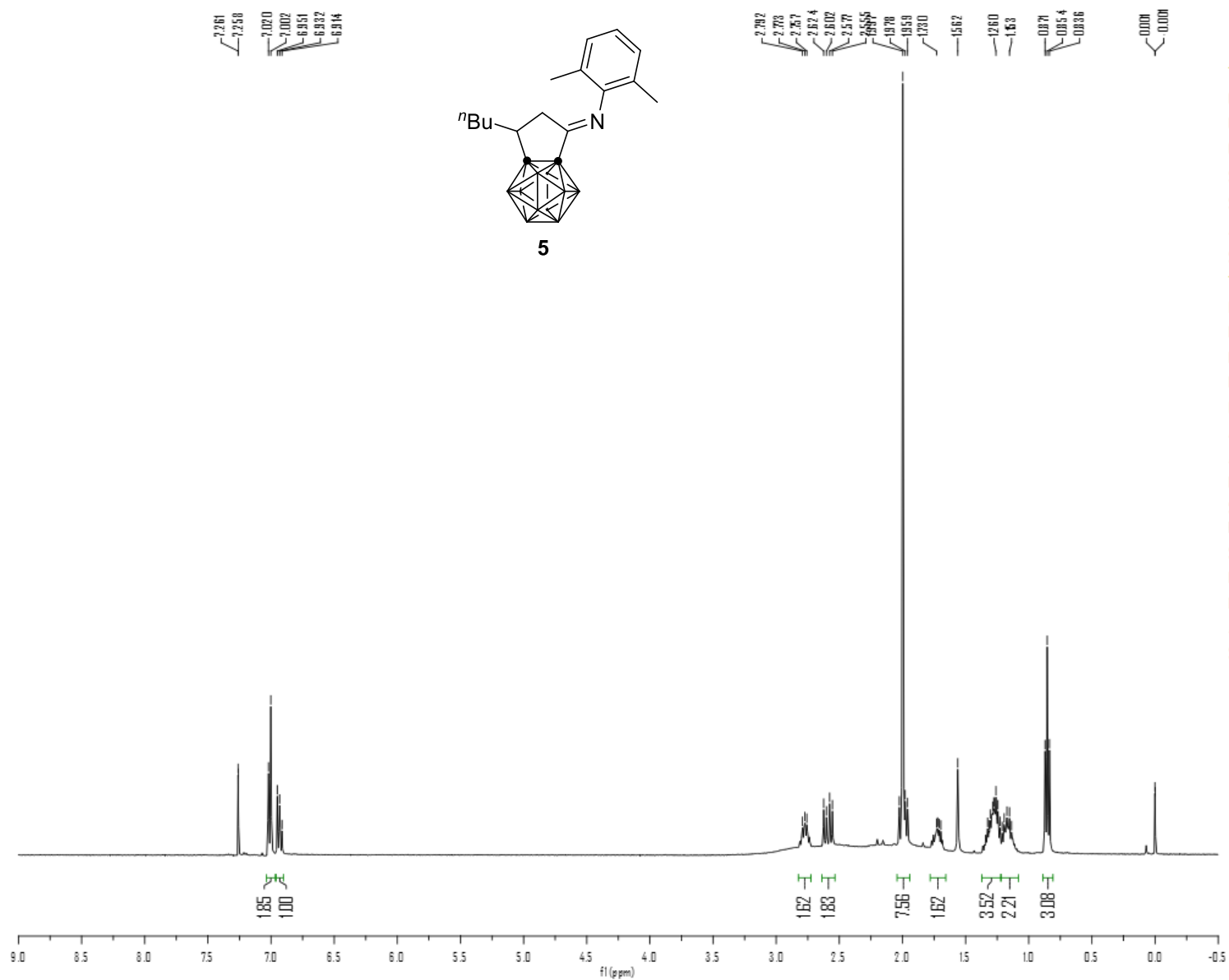
46.40
6.62
7.255
8.631
10.006



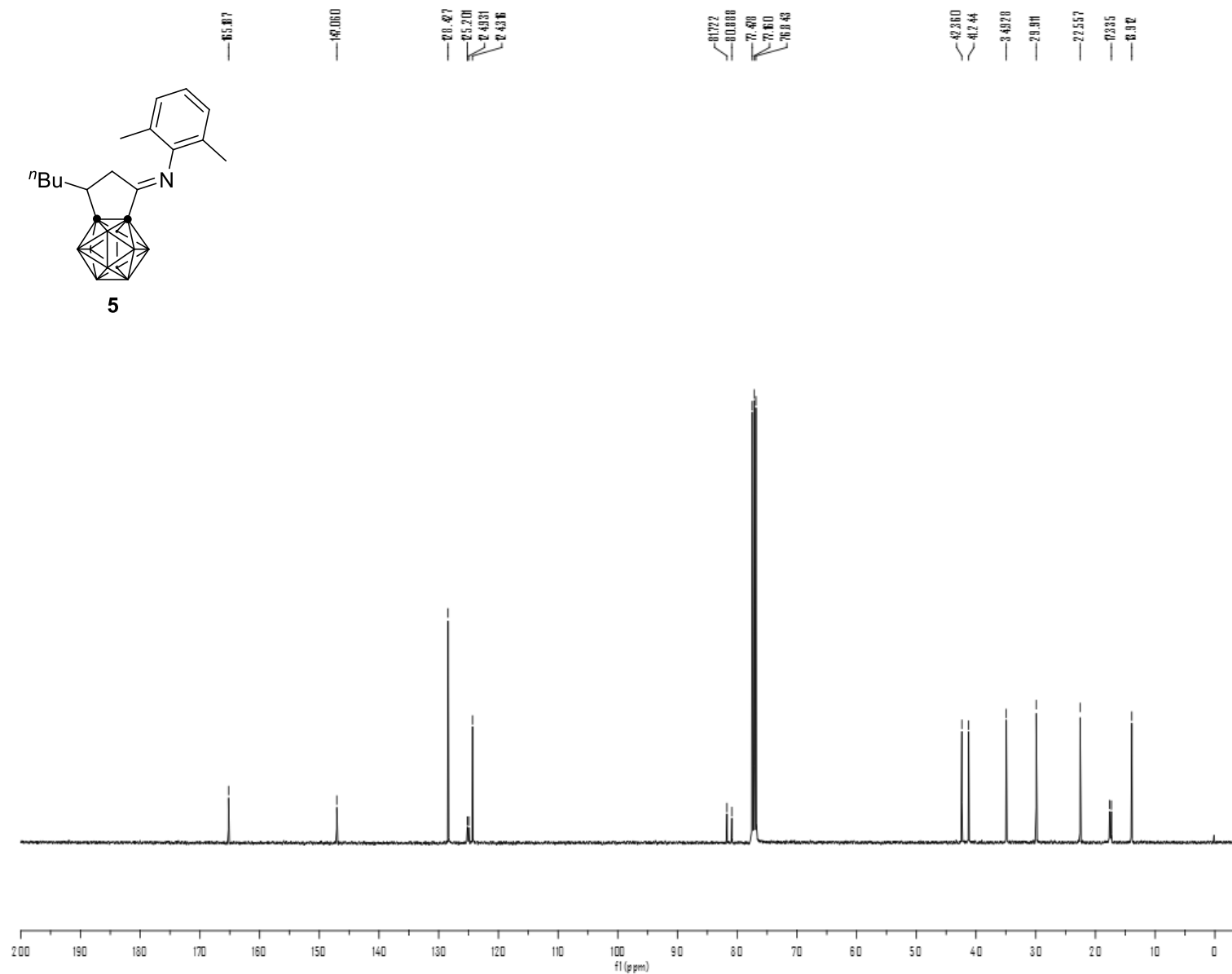
Parameter	Value
Data File Name	C:/Users/culchunxiao/Desktop/b-cxx-7-10 8-3/pdata/1/ 1r
Title	Desktop
Comment	
Origin	UXMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	Pyr
Temperature	300.0
Pulse Sequence	aring.1g
Number of Scans	1221
Receiver Gain	512
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.5112
Acquisition Date	2017-05-19T19:22:30
Modification Date	2017-05-19T13:32:00
Spectrometer Frequency	128.38
Spectral Width	32051.3
Lowest Frequency	-16404.2
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



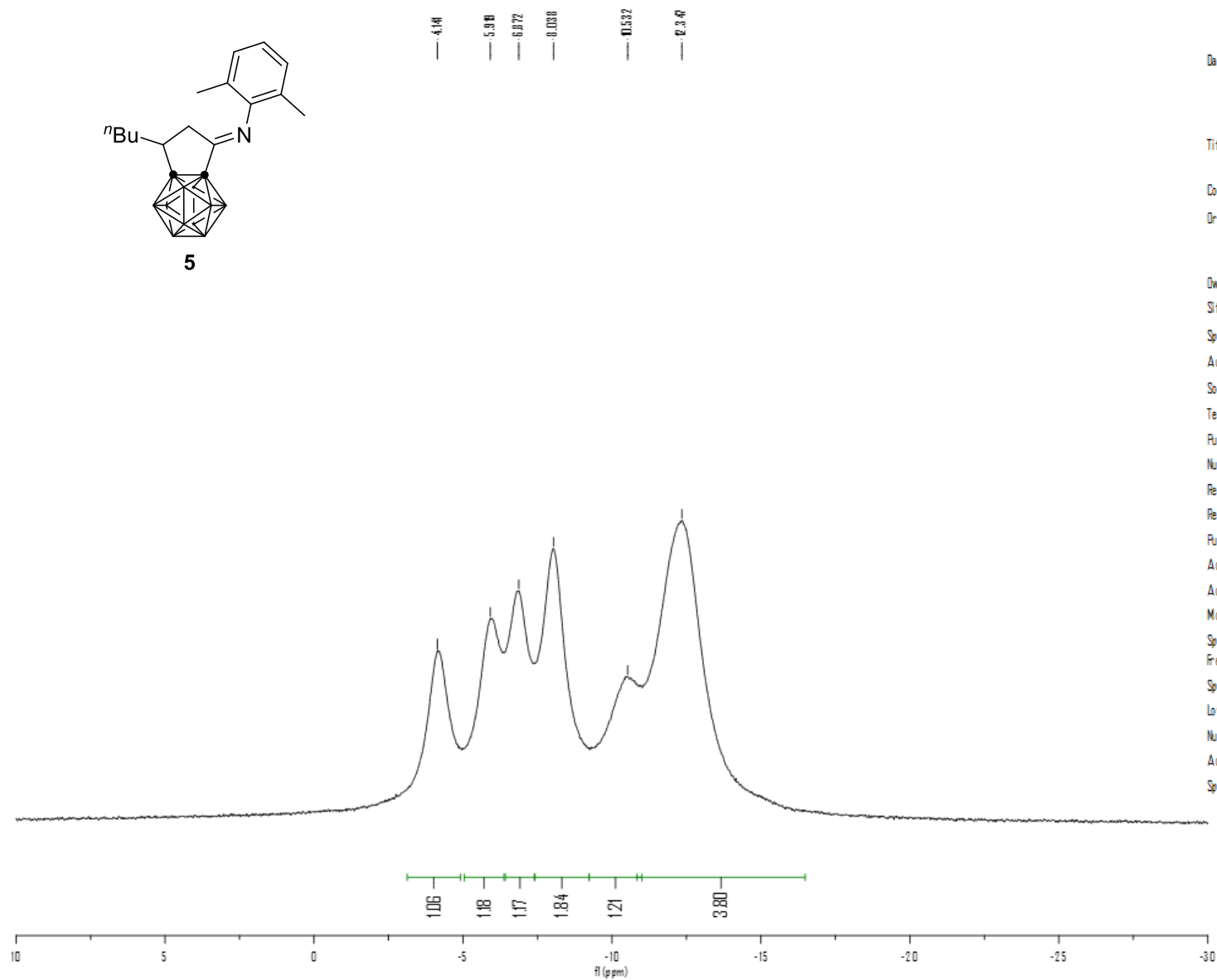
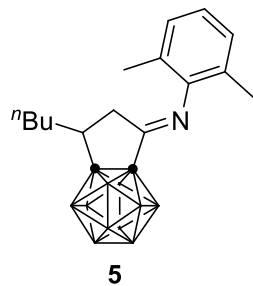
Parameter	Value
Title	ccx-7-10 3-3-P
Comment	wft.aph.cdc.f
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	pyridine
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	72
Receiver Gain	50
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2017-05-18T22:17:22
Modification Date	2017-05-18T14:20:00
Spectrometer Frequency	161.81
Spectral Width	89285.7
Lowest Frequency	-41333.8
Nucleus	31P
Acquired Size	89286
Spectral Size	262144



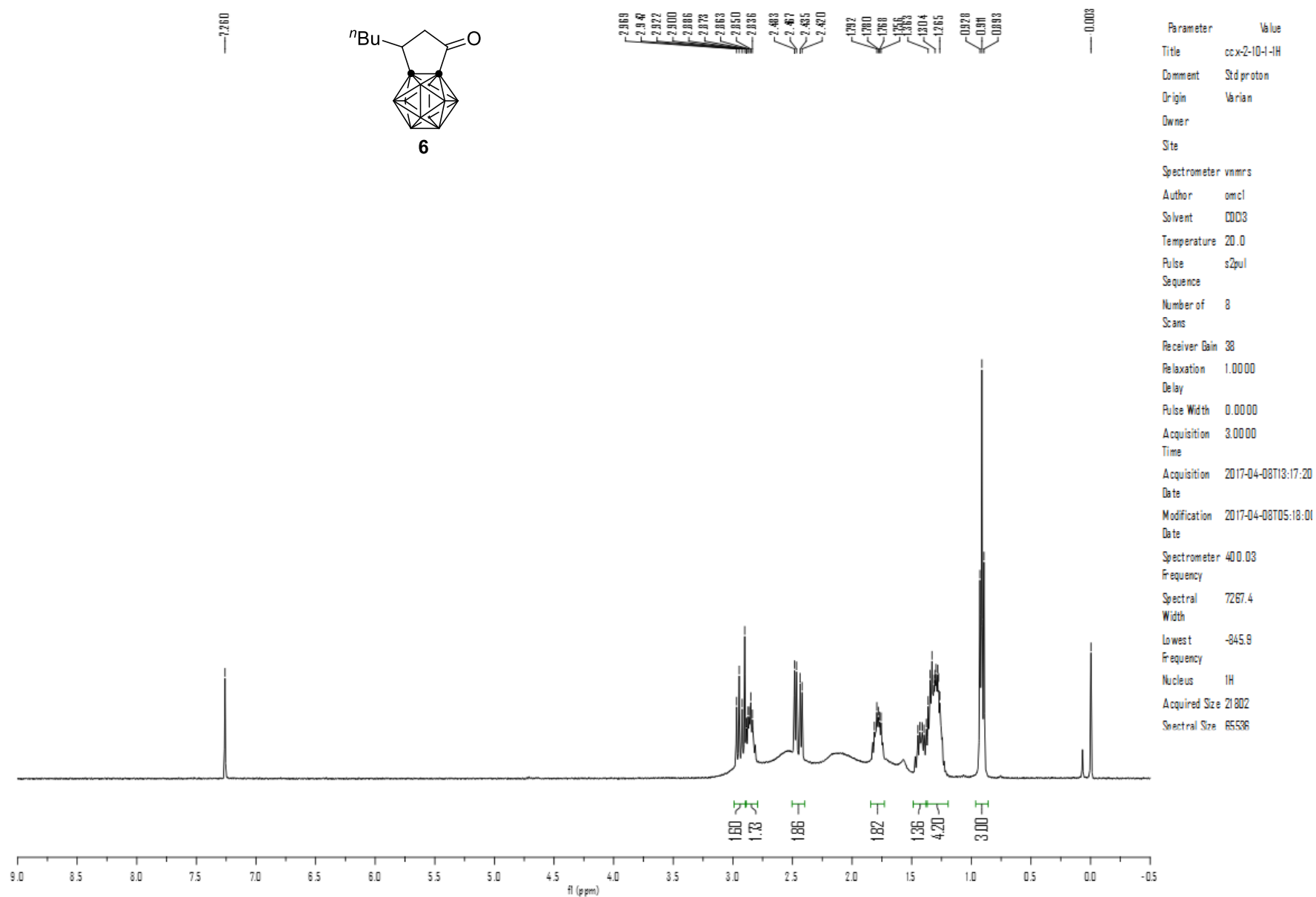
Parameter	Value
Title	ccx-7-100-3-1-1
Comment	xcx-Sc12
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	42
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-05-10T00:01:36
Modification Date	2017-05-09T16:02:00
Spectrometer Frequency	369.72
Spectral Width	7183.9
Lowest Frequency	-793.9
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

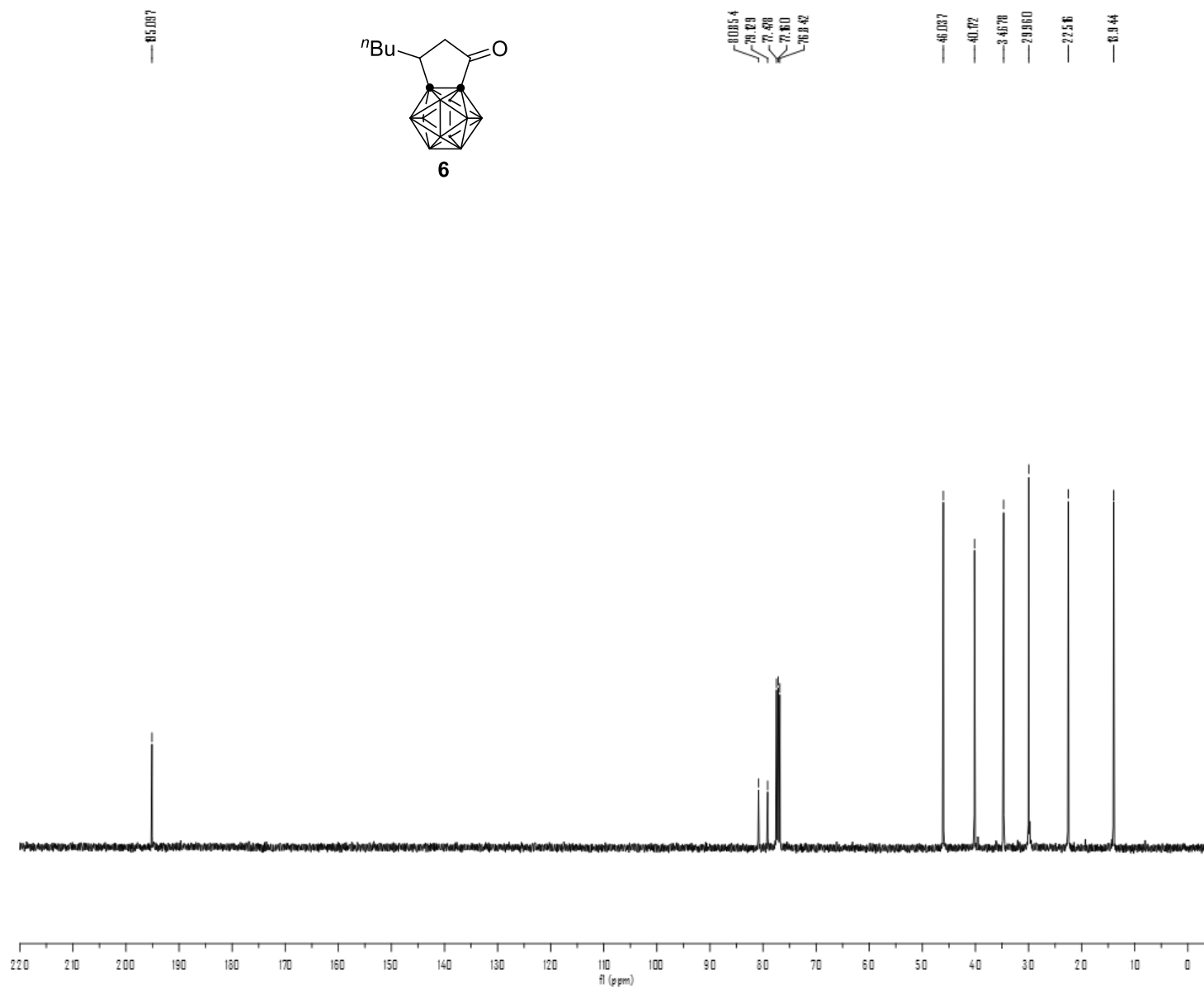


Parameter	Value
Title	ccx-7-10 0-31-10C
Comment	lxj-2-54-C-H
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	11864
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.2845
Acquisition Date	2017-05-12T22:26:08
Modification Date	2017-05-12T22:02:00
Spectrometer Frequency	100.52
Spectral Width	25510.2
Lowest Frequency	-1265.6
Nucleus	13C
Acquired Size	32768
Spectral Size	65536

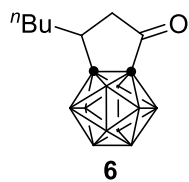


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-ccx-7-10-3-2-a/1/pdata/1/1r
Title	20120606-ccx-7-10-3-2-a
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.lgy
Number of Scans	200
Receiver Gain	256
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.3195
Acquisition Date	2017-05-08T21:34:41
Modification Date	2017-05-08T15:03:14
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-25985.1
Nucleus	13C
Acquired Size	16384
Spectral Size	32768

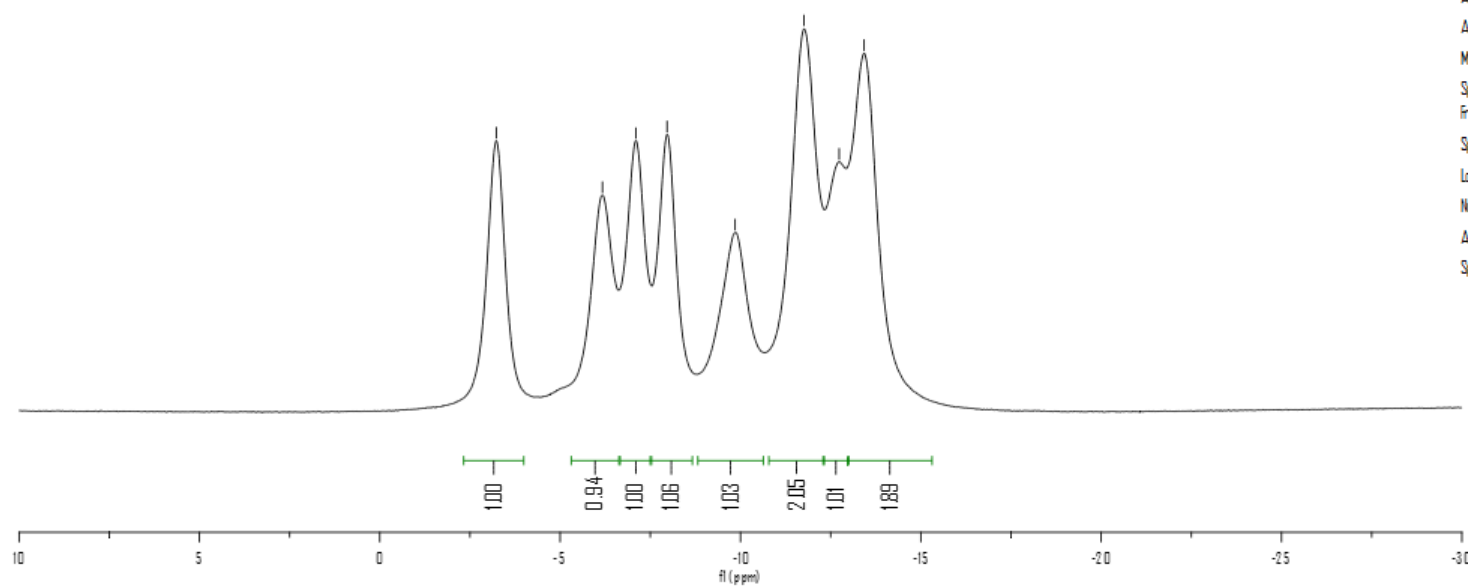




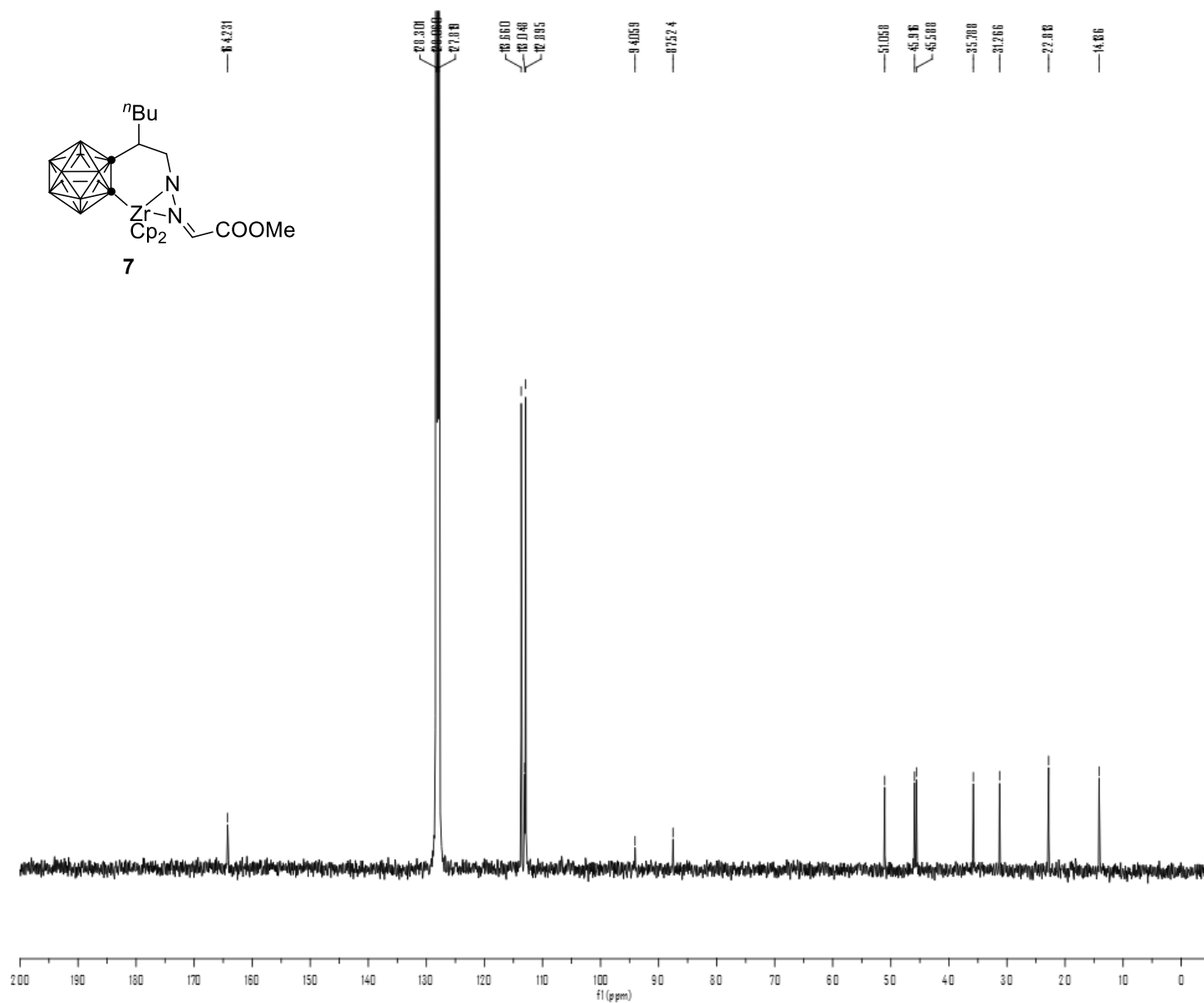
Parameter	Value
Title	ccx-2-38-1C
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	332
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-04-08T22:50:18
Modification Date	2017-04-08T15:03:00
Spectrometer Frequency	100.60
Spectral Width	26041.7
Lowest Frequency	-1690.8
Nucleus	^{13}C
Acquired Size	33987
Spectral Size	131072



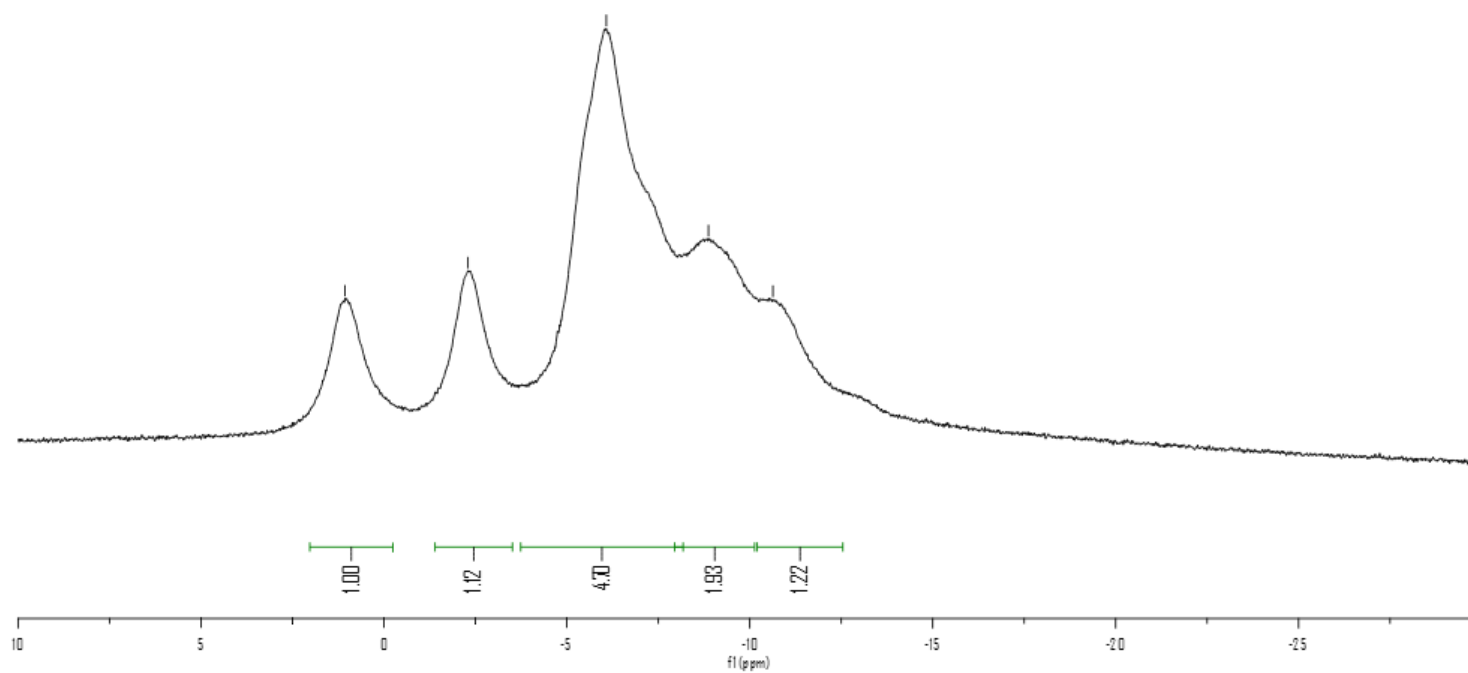
— 3.229 — 6.474 — 7.100 — 7.963 — 9.052 — 11.763 — 12.287 — 13.429

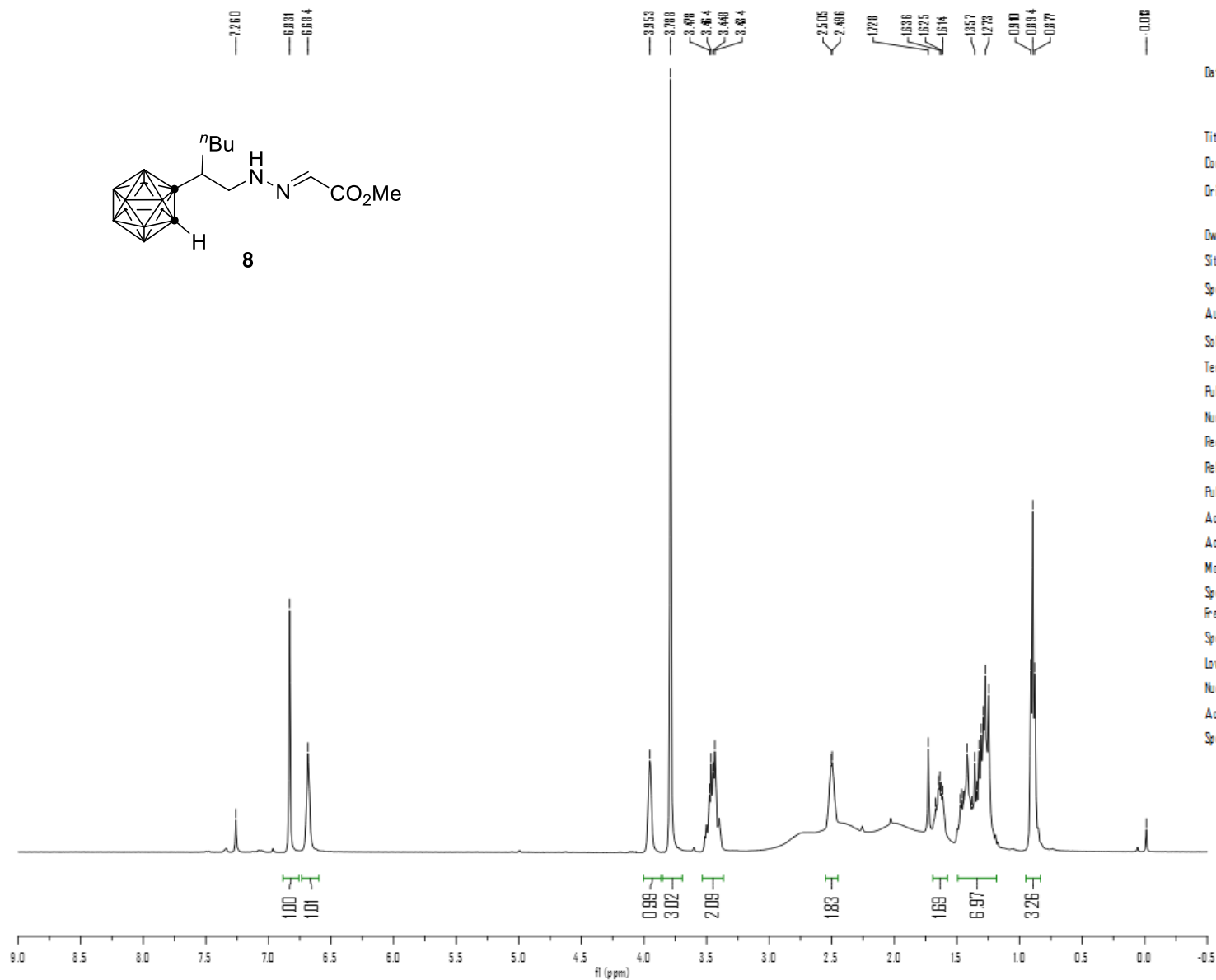


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/b-cxx-2-36-1 (1)/pdata/1/1r
Title	Desktop
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	767
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.3165
Acquisition Date	2015-01-09T17:36:38
Modification Date	2015-01-09T10:36:00
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-17838.7
Nucleus	1H
Acquired Size	16384
Spectral Size	32768

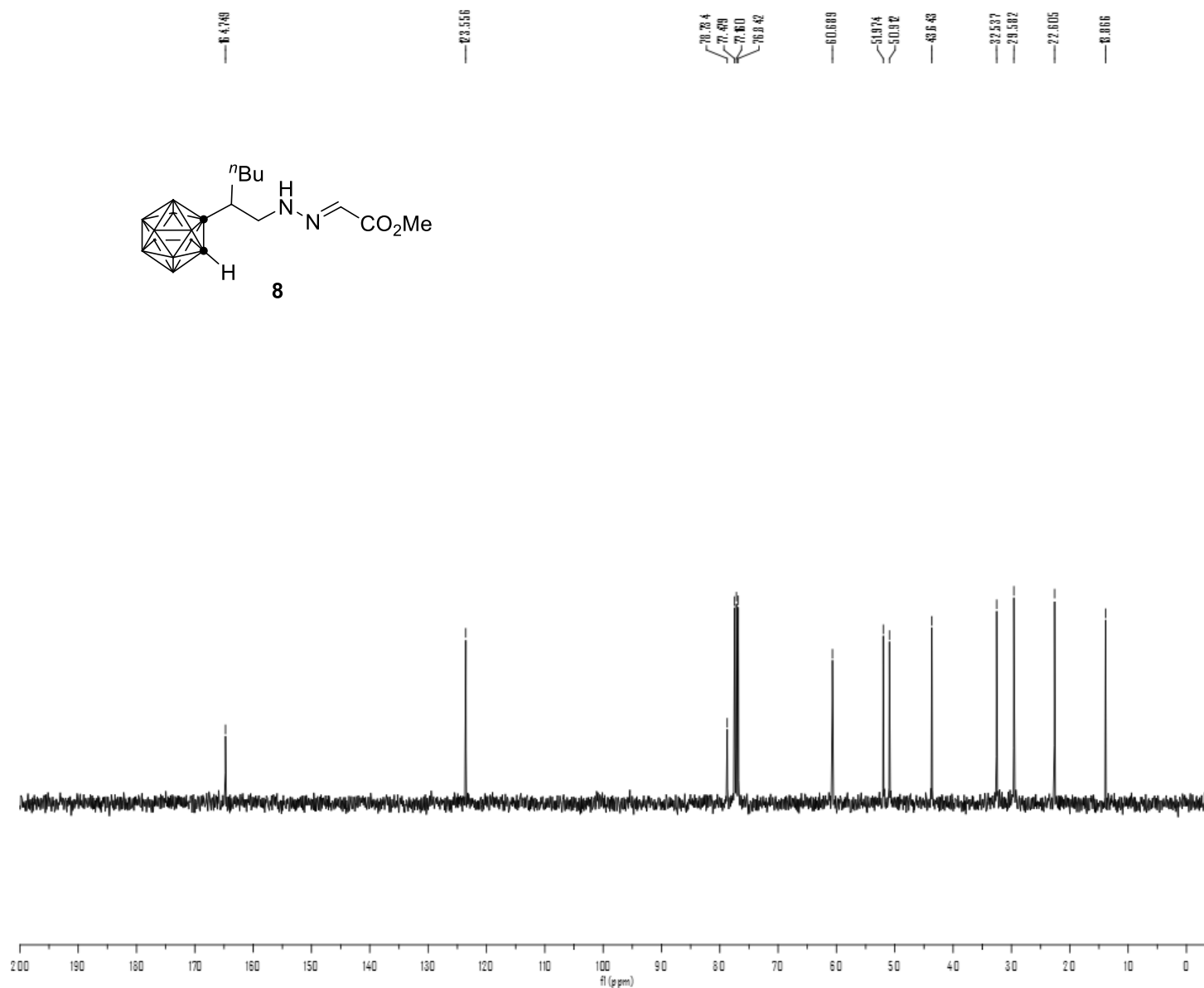


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/ccc-cxx-4-75-1/pdata/1/1r
Title	c13
Comment	
Origin	UXNM R. Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	1800
Receiver Gain	16384
Relaxation Delay	3.0000
Pulse Width	6.0000
Acquisition Time	0.4654
Acquisition Date	2015-08-15T18:35:42
Modification Date	2015-08-15T14:38:00
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-8871.5
Nucleus	13C
Acquired Size	16384
Spectral Size	65536

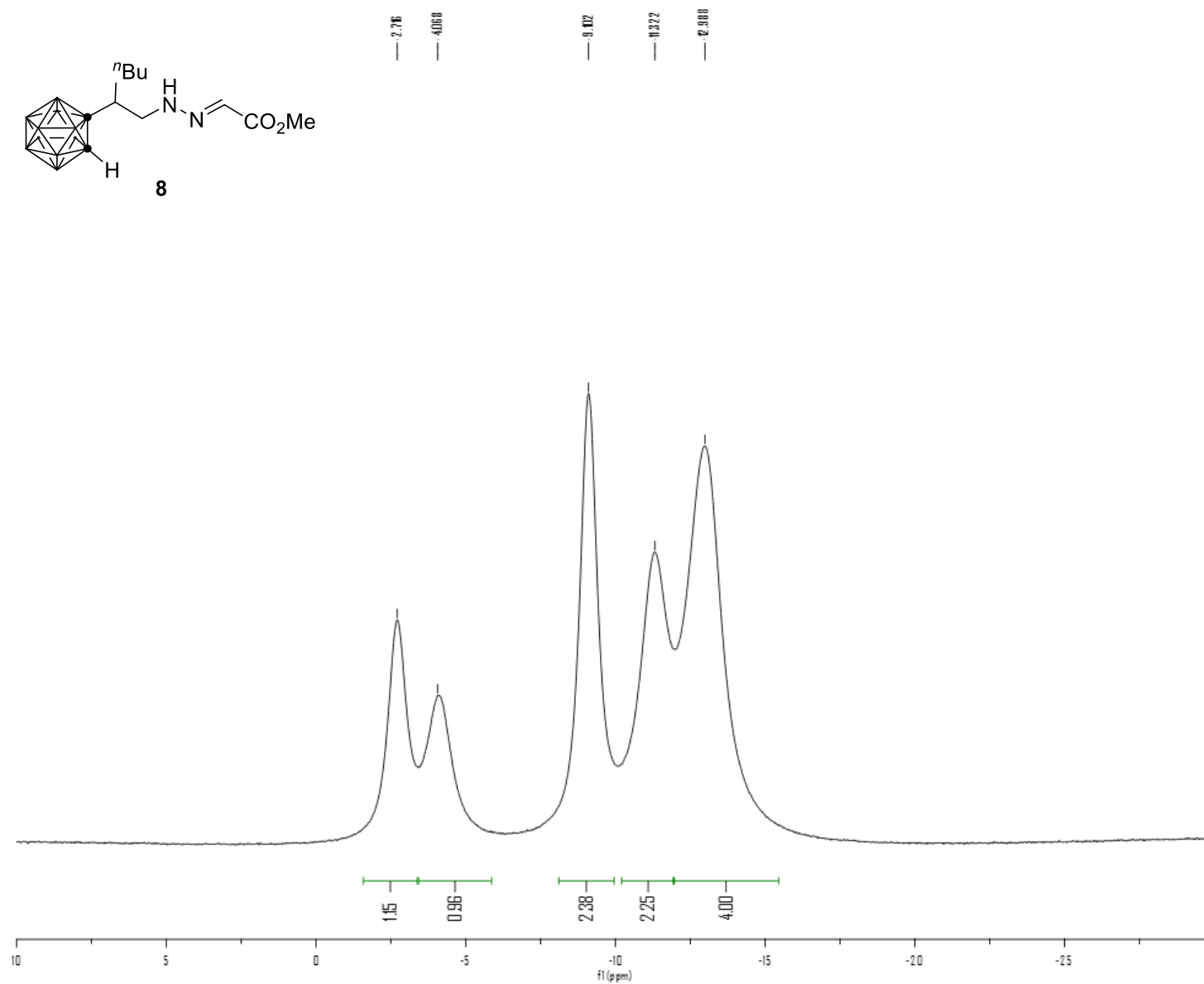
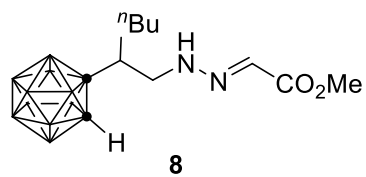
S27



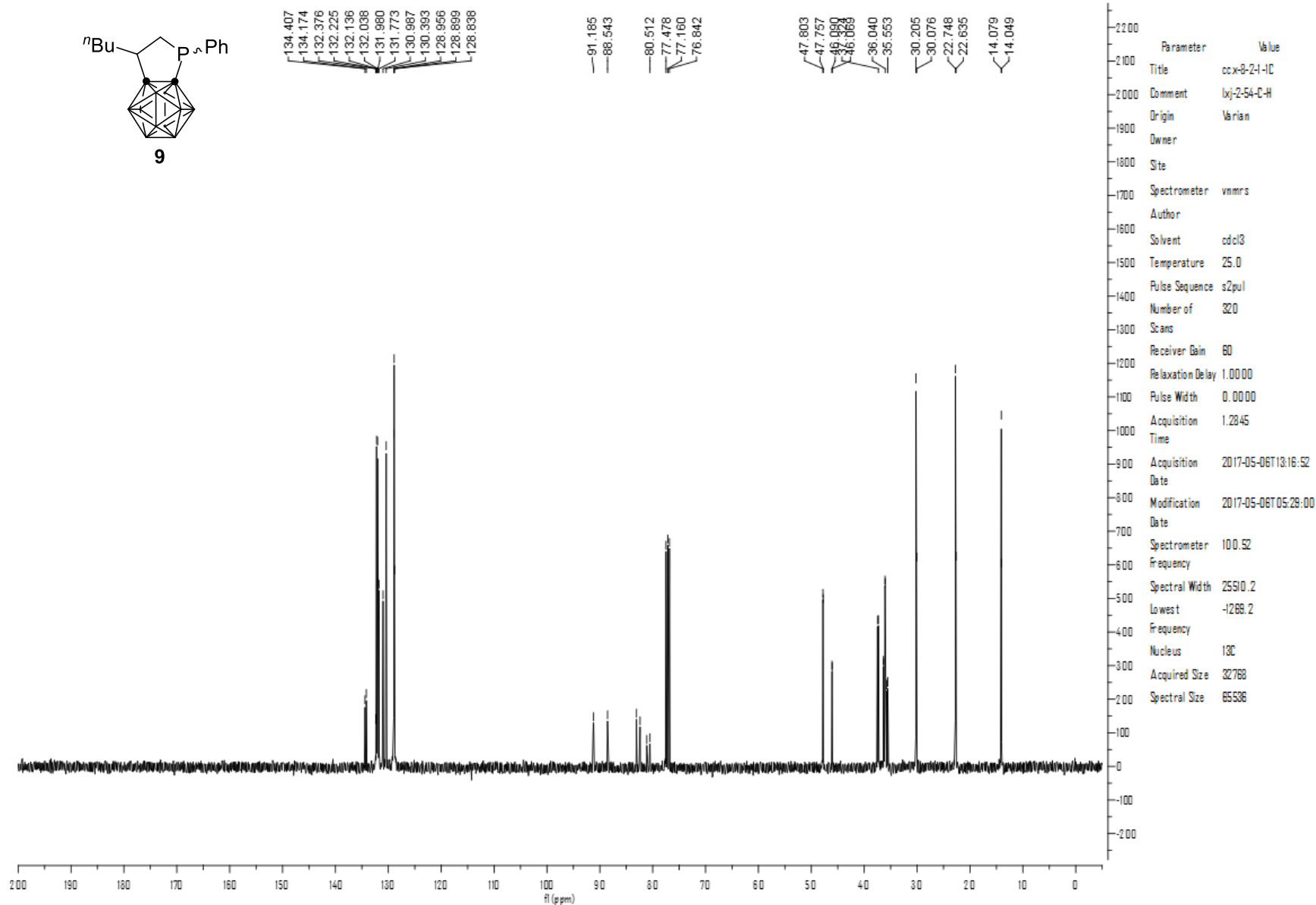
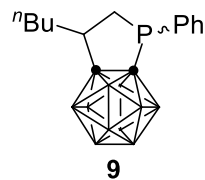
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/h-cx-4-85-1/pdata/1/1r
Title	Desktop
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl ₃
Temperature	30.0
Pulse Sequence	zg
Number of Scans	8
Receiver Gain	32
Relaxation Delay	2.0000
Pulse Width	4.0000
Acquisition Time	1.3631
Acquisition Date	2015-07-03T20:28:10
Modification Date	2015-07-03T14:28:00
Spectrometer	400.13
Frequency	
Spectral Width	12019.2
Lowest Frequency	-4504.8
Nucleus	¹ H
Acquired Size	16384
Spectral Size	32768

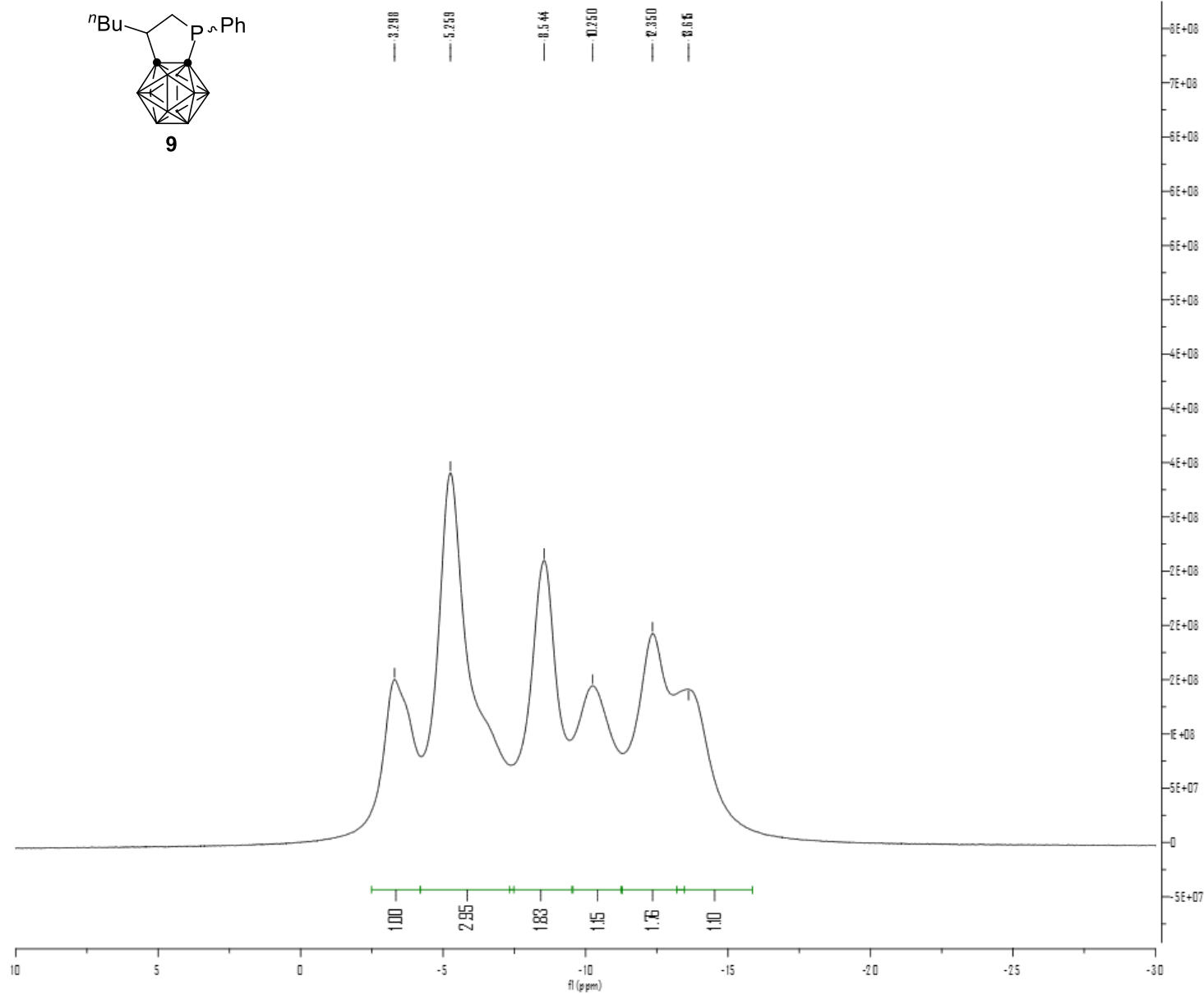
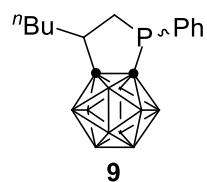


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/c-cx-4-85-1/pdata/1/ 1r
Title	c13
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	zgdc
Number of Scans	223
Receiver Gain	16384
Relaxation Delay	2.0000
Pulse Width	6.0000
Acquisition Time	0.4654
Acquisition Date	2015-07-03T20:34:08
Modification Date	2015-07-03T14:42:00
Spectrometer Frequency	100.61
Spectral Width	35211.3
Lowest Frequency	-6503.5
Nucleus	13C
Acquired Size	16384
Spectral Size	65536

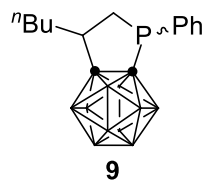


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/b-cx-4-65-1/pdata/1/1r
Title	Desktop
Comment	
Origin	UXNMR Bruker
	Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	DMSO
Temperature	300.0
Pulse Sequence	aring1g
Number of Scans	615
Receiver Gain	32
Relaxation Delay	0.0000
Pulse Width	13.4000
Acquisition Time	0.3165
Acquisition Date	2015-07-03T21:37:58
Modification Date	2015-07-03T15:40:00
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-17820.9
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

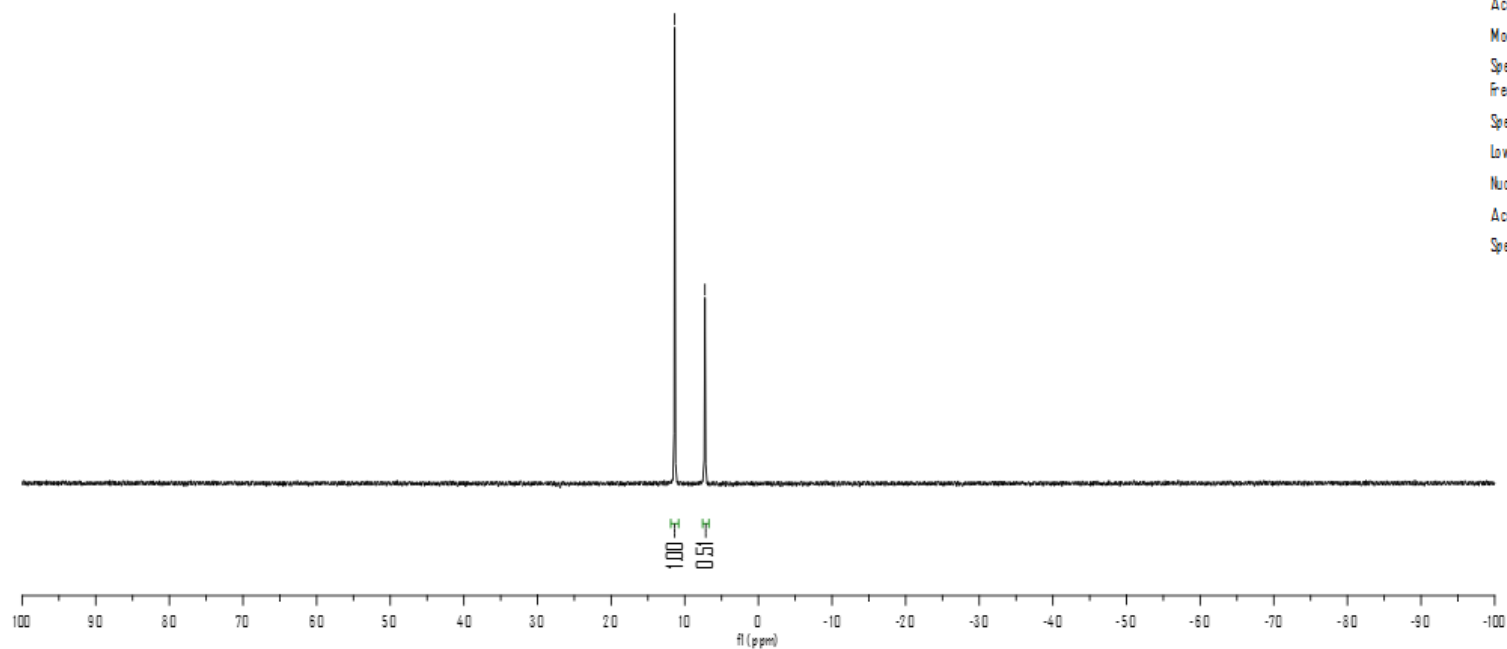




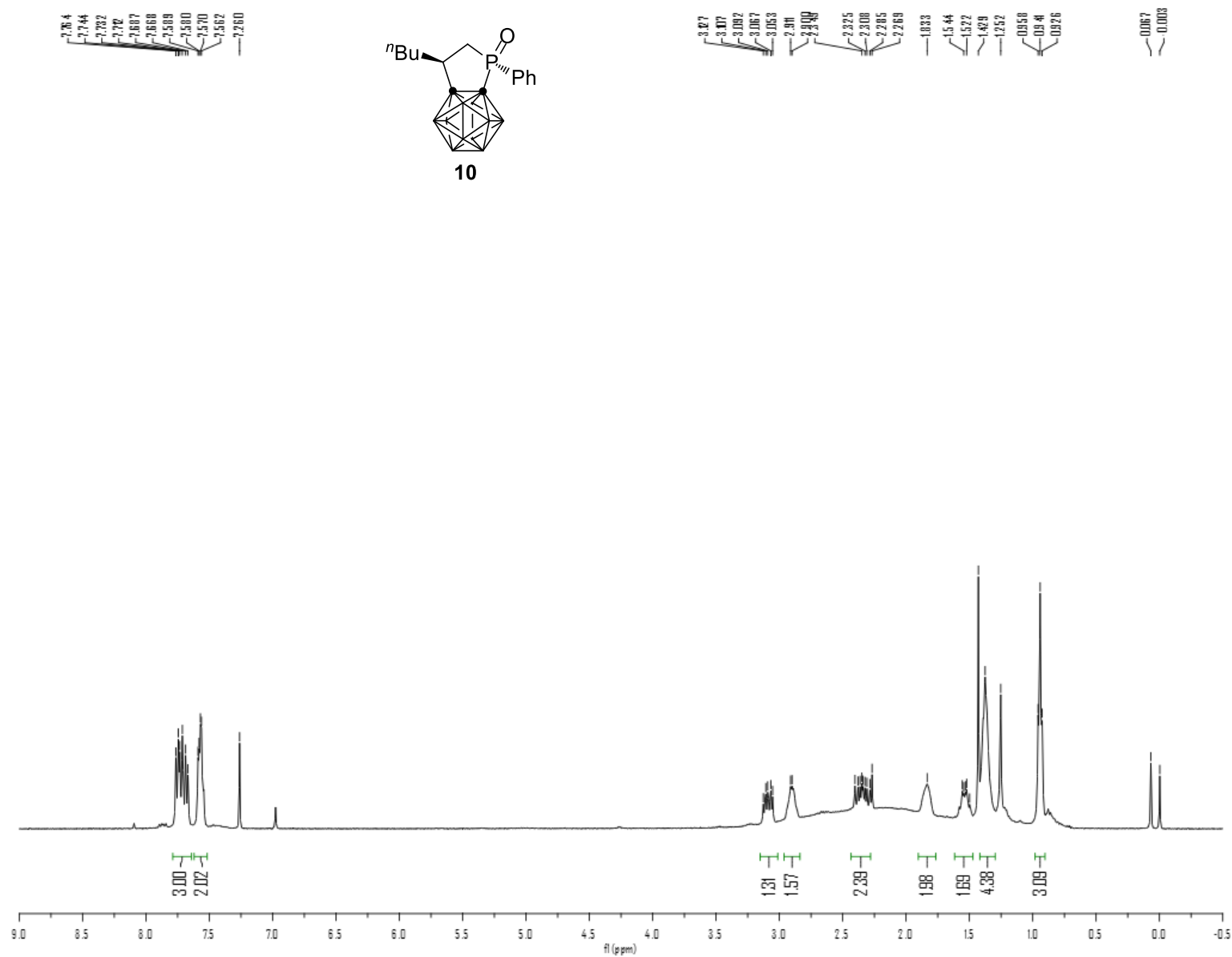
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-ccx-9-2-1/1/ pdata/1/ 1r
Title	20120606-ccx-9-2-1
Comment	
Origin	UXNM/R Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.lgy
Number of Scans	200
Receiver Gain	161
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.3185
Acquisition Date	2017-05-08T21:45:15
Modification Date	2017-05-08T15:03:06
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-25685.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



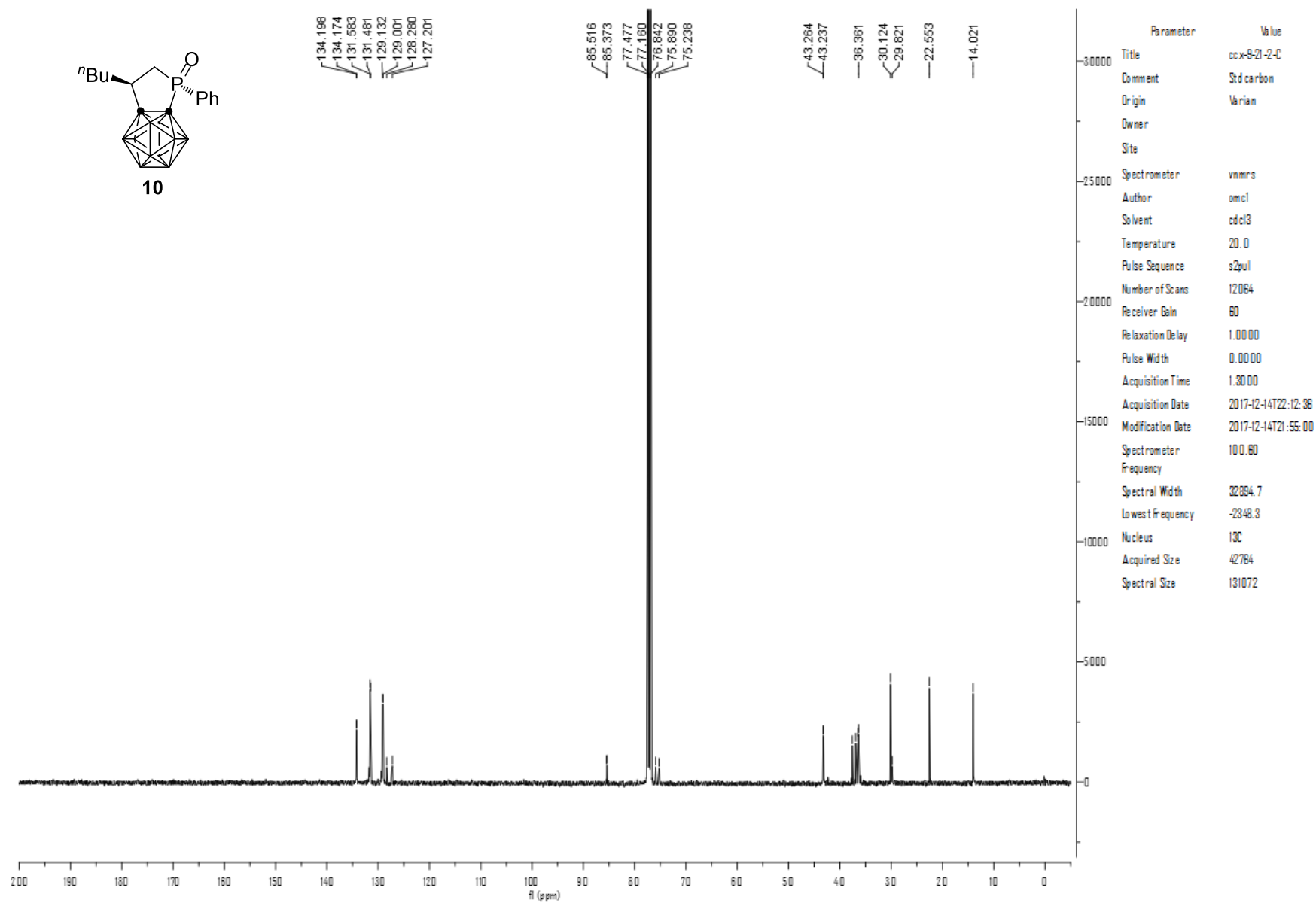
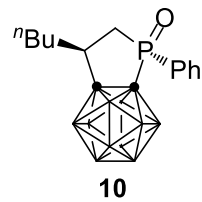
103.4
72.66

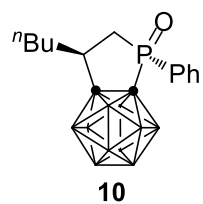


Parameter	Value
Title	cox-9-2-1-1-P
Comment	STANDARD CARBON PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	nmrs
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	16
Receiver Gain	50
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2017-05-06T13:29:20
Modification Date	2017-05-06T05:30:00
Spectrometer	161.81
Frequency	
Spectral Width	73528.4
Lowest Frequency	-32412.0
Nucleus	31P
Acquired Size	73528
Spectral Size	262144

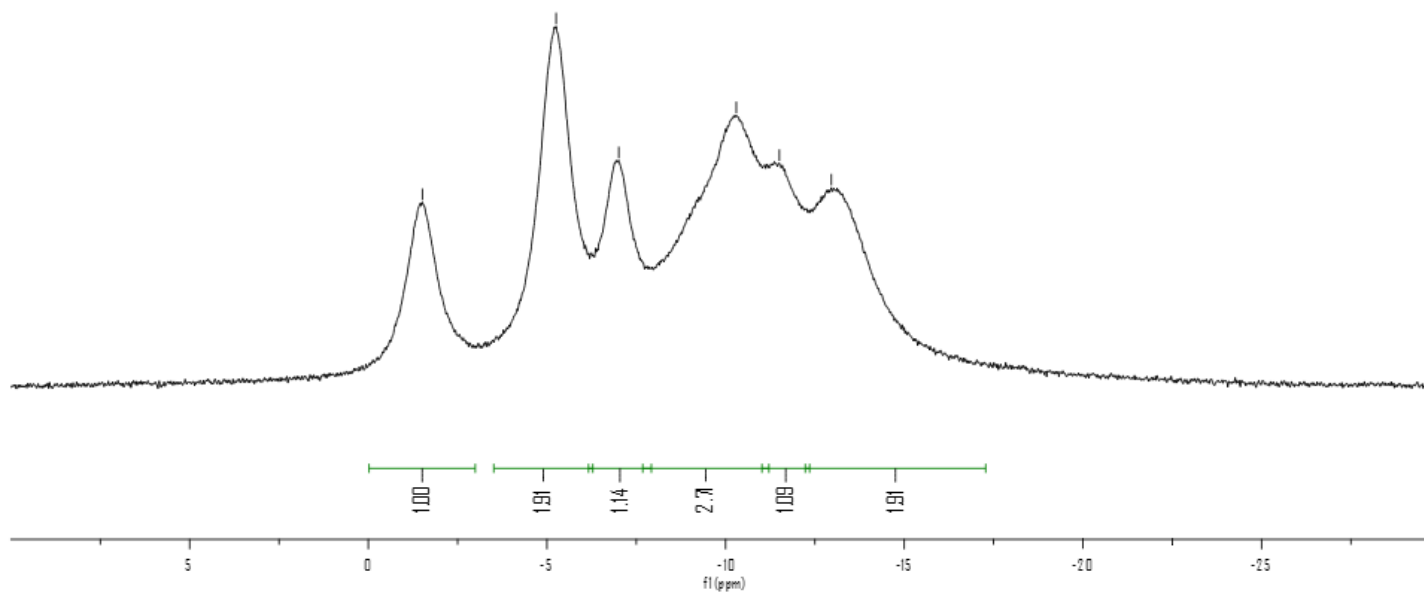


Parameter	Value
Title	ccx-8-15-1-54-80
Comment	xc-c-Sc12
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	CDCl3
Temperature	25.0
Pulse	s2pul
Sequence	
Number of Scans	16
Receiver Gain	32
Relaxation	1.0000
Delay	
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-05-17T12:26:10
Modification Date	2017-05-17T04:27:00
Spectrometer	389.72
Frequency	
Spectral Width	7183.9
Lowest Frequency	-793.5
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

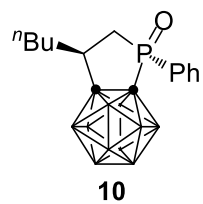




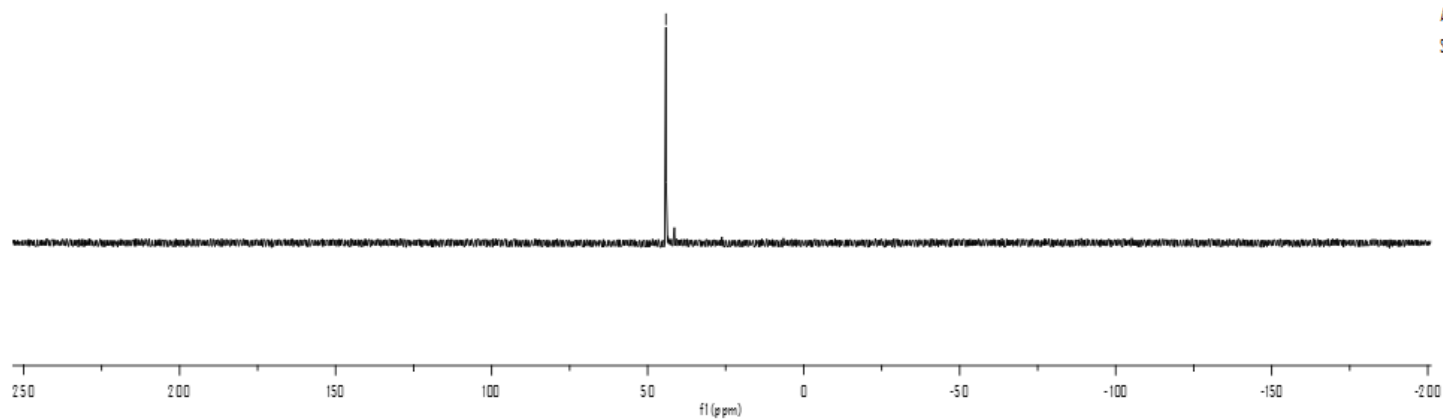
Chemical shifts (ppm): 13.6, 5.256, 7.00, 10.300, 11.505, 2.960



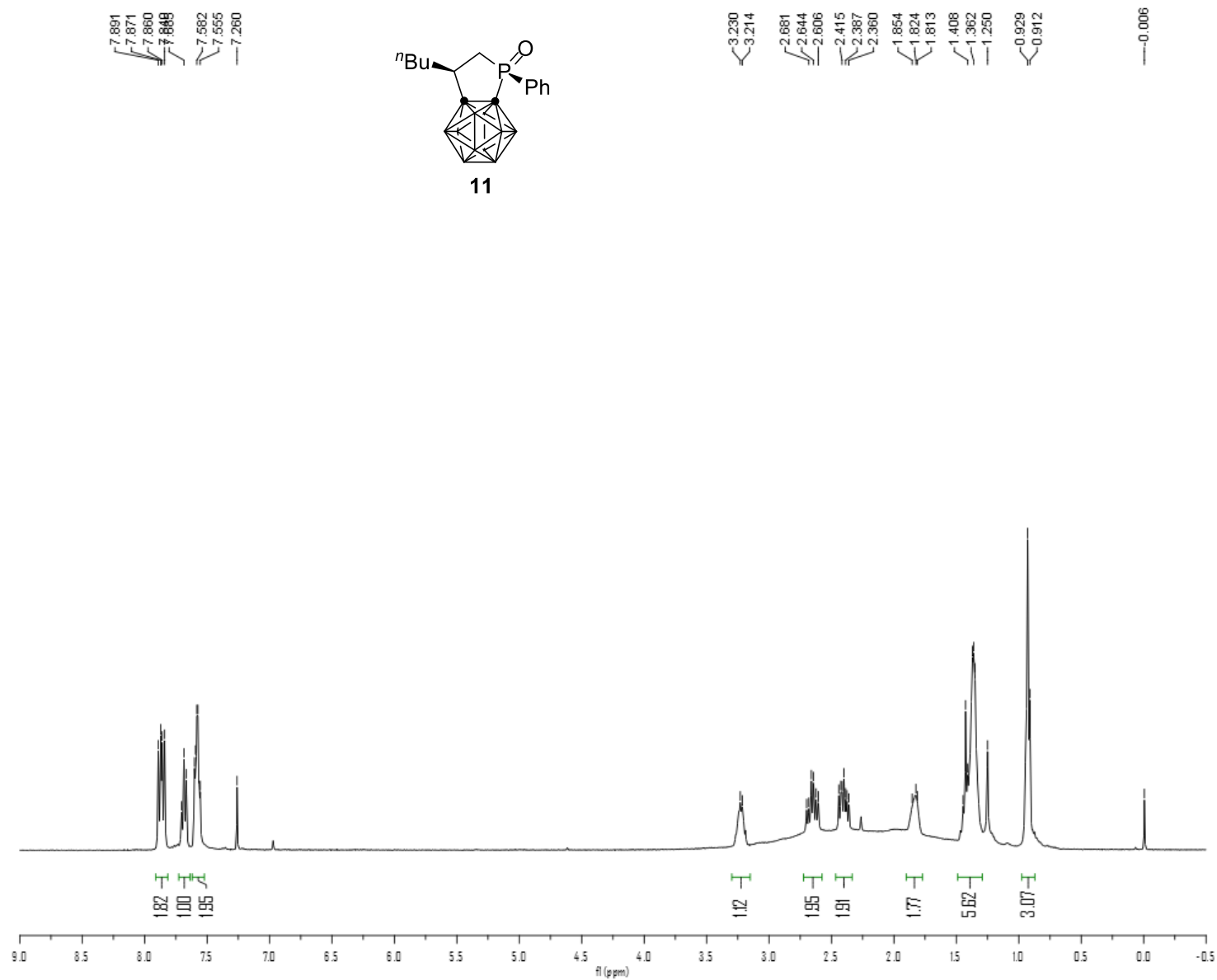
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-ccx-8-15-1-54-60/1/ pdata/1/ 1r
Title	20120606-ccx-8-15-1-54-60
Comment	
Origin	UXNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	181
Receiver Gain	322
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.3165
Acquisition Date	2017-05-18T19:05:07
Modification Date	2017-05-18T13:17:44
Spectrometer	128.38
Frequency	
Spectral Width	51282.1
Lowest Frequency	-25883.4
Nucleus	1H
Acquired Size	16384
Spectral Size	32768



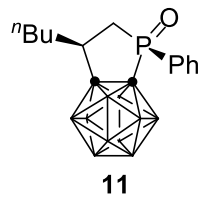
—44.154



Parameter	Value
Title	ccx-8-154-54-80-PP
Comment	STANDARD CARBON PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	52
Receiver Gain	50
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2017-05-18T23:00:28
Modification Date	2017-05-18T15:03:00
Spectrometer Frequency	161.81
Spectral Width	73528.4
Lowest Frequency	-32528.7
Nucleus	^{31}P
Acquired Size	73528
Spectral Size	262144



Parameter	Value
Title	ccx-8-15-1-24-30 HH
Comment	
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	34
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-05-30T20:57:31
Modification Date	2017-05-30T12:58:00
Spectrometer Frequency	399.72
Spectral Width	6410.3
Lowest Frequency	-806.8
Nucleus	1H
Acquired Size	19231
Spectral Size	65536

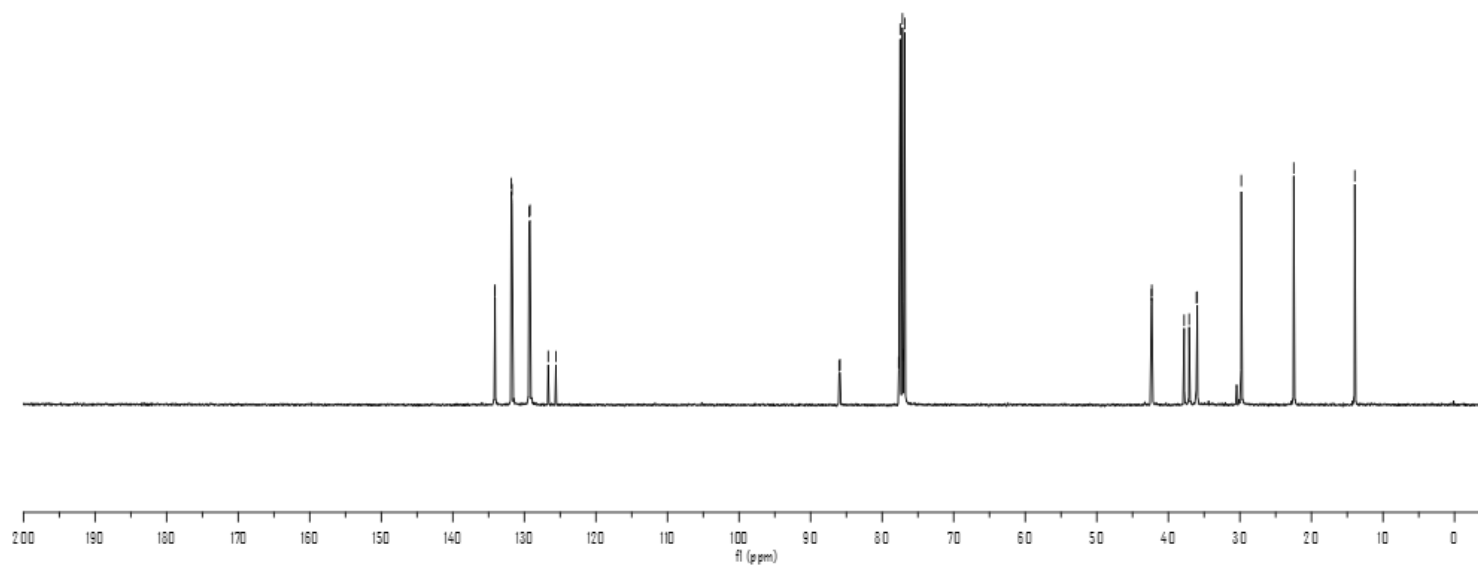


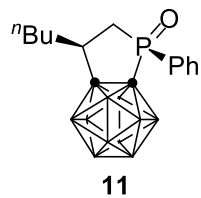
134.130
134.101
131.832
131.734
129.343
129.214
126.670
125.590

86.017
85.884
77.682
77.478
77.160
77.060
76.843

42.352
42.317
37.090
35.953
29.801
22.468
13.940

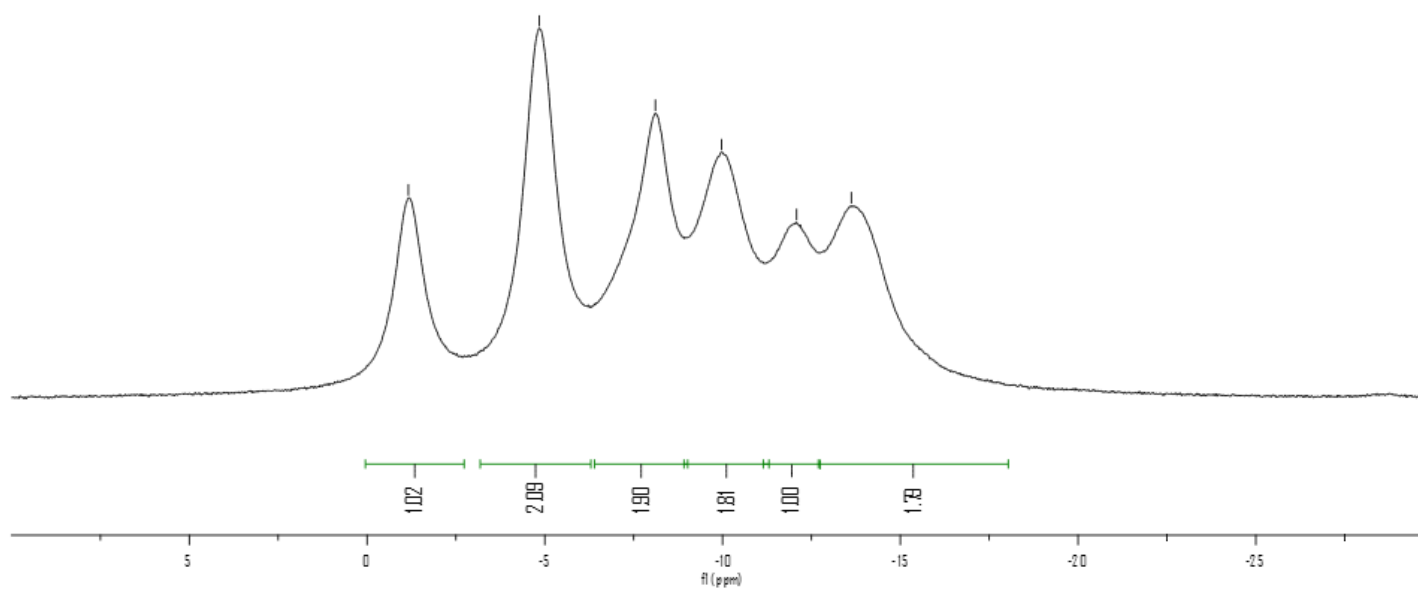
Parameter	Value
Title	ccx-8-15-1-24-30-cc
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	13872
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-05-30T21:54:04
Modification Date	2017-05-30T22:51:00
Spectrometer Frequency	100.60
Spectral Width	24509.8
Lowest Frequency	-1677.2
Nucleus	¹³ C
Acquired Size	31875
Spectral Size	65536



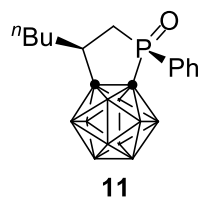


Chemical shifts (ppm) indicated above the spectrum:

- 1.163
- 4.841
- 8.110
- 9.970
- 12.083
- 13.622

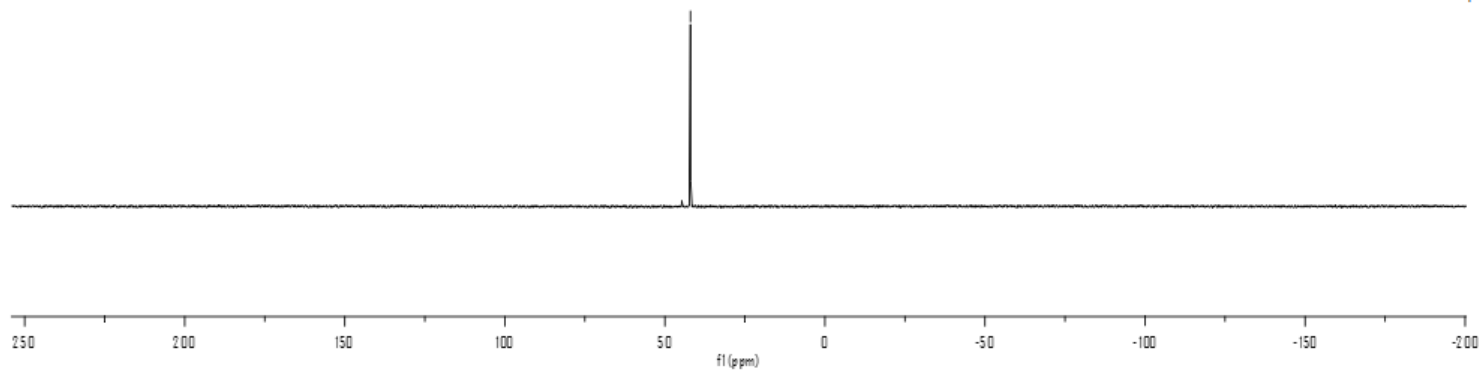


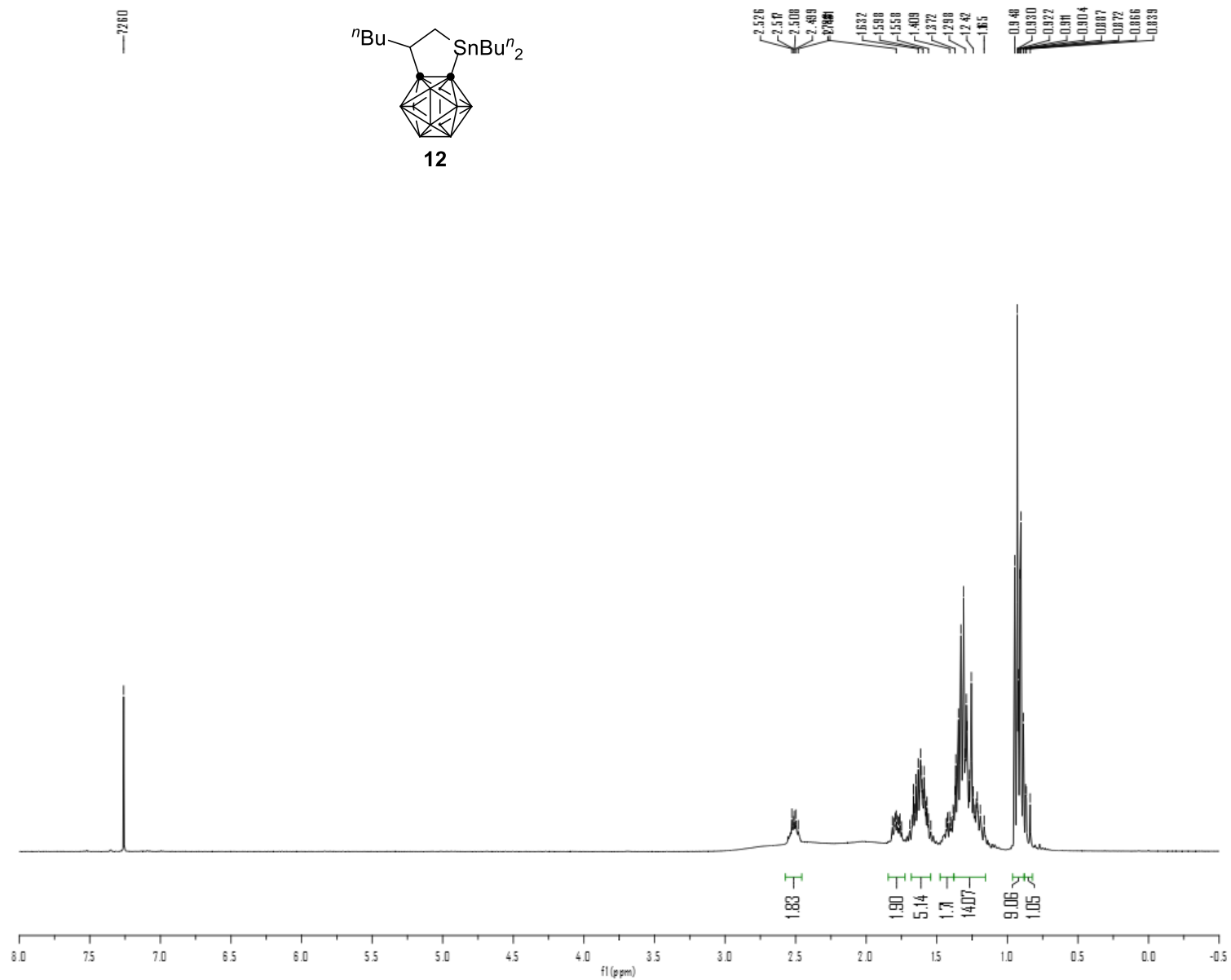
Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-ccx-8-15-1-24-30/1/pdata/1/1r
Title	20120606-ccx-8-15-1-24-30
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.jgy
Number of Scans	213
Receiver Gain	203
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.3195
Acquisition Date	2017-05-18T19:07:36
Modification Date	2017-05-18T13:17:38
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-25983.4
Nucleus	11B
Acquired Size	16384
Spectral Size	32768



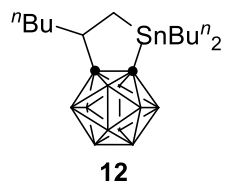
42.014

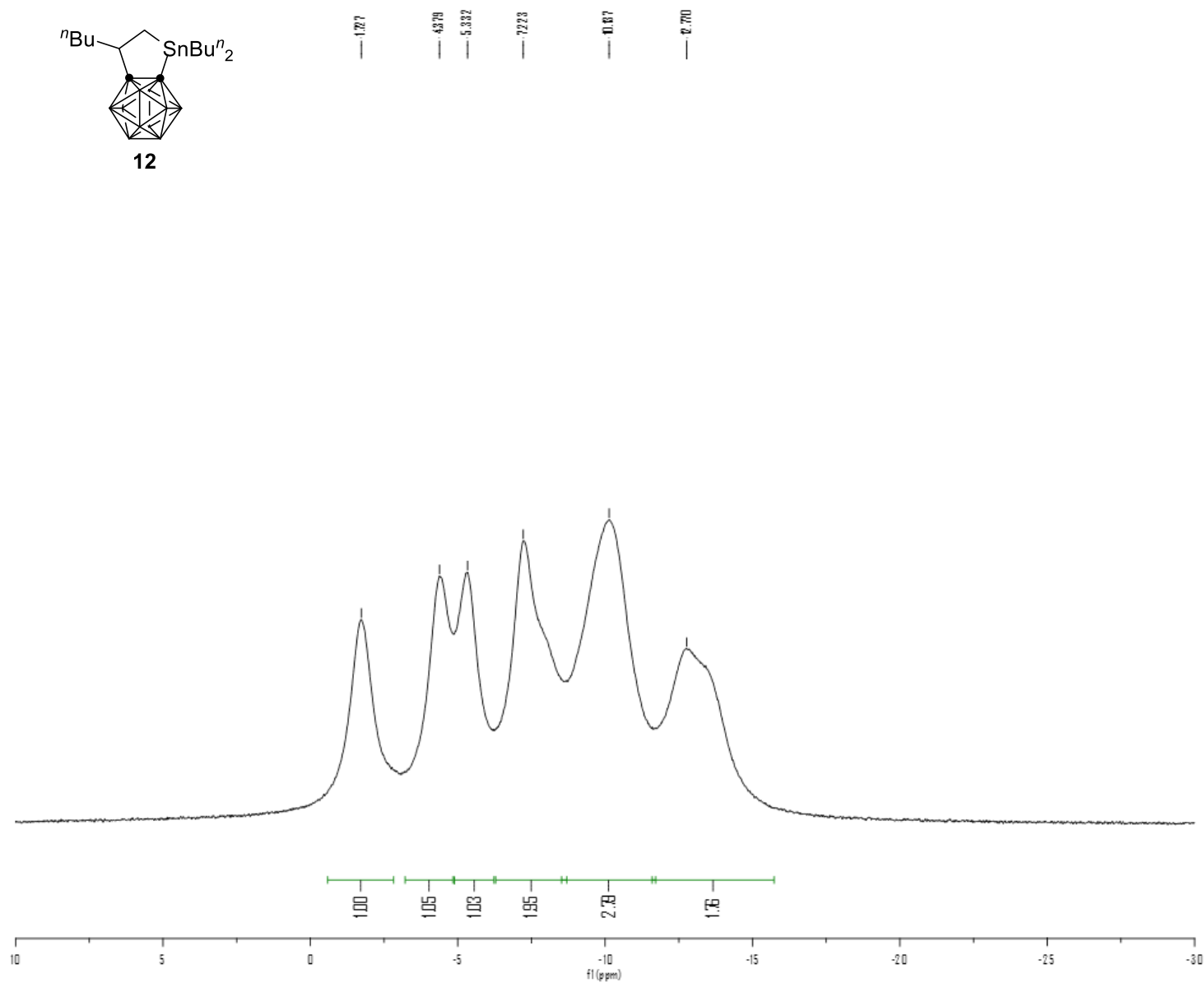
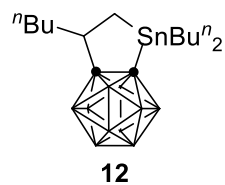
Parameter	Value
Title	ccx-8-15-1-24-30-PPP
Comment	STANDARD CARBON PARAMETERS
Origin	Varian
Owner	
Site	
Spectrometer	nmr-s
Author	
Solvent	cdcl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	76
Receiver Gain	50
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.0000
Acquisition Date	2017-05-30T20:58:54
Modification Date	2017-05-30T13:01:00
Spectrometer Frequency	161.81
Spectral Width	73529.4
Lowest Frequency	-32412.0
Nucleus	31P
Acquired Size	73529
Spectral Size	262144



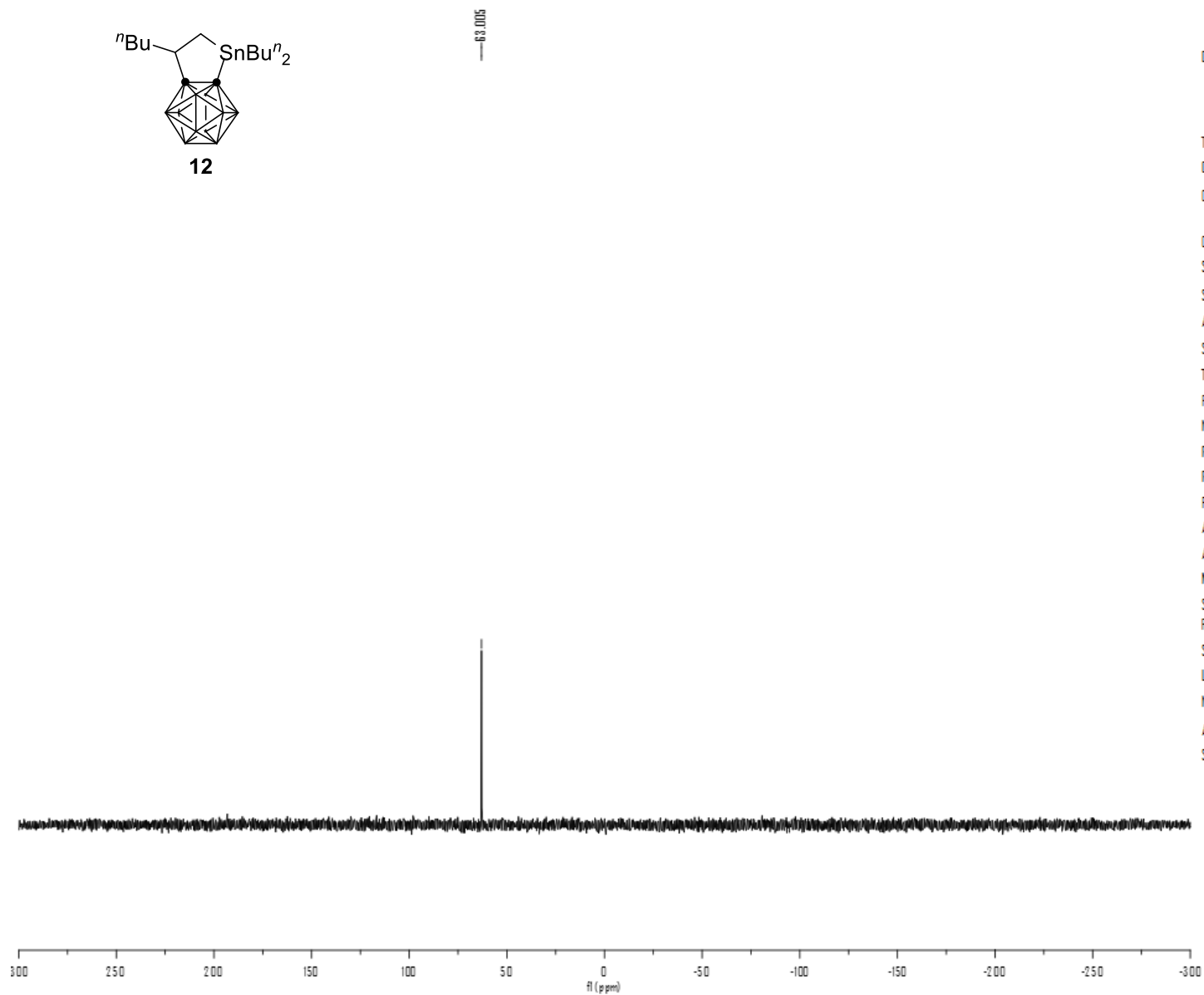
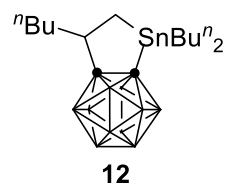


Parameter	Value
Title	ccx-8-9-1
Comment	xc-c-Sc(2)
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	
Solvent	CDCl3
Temperature	25.0
Pulse Sequence	s2pul
Number of Scans	12
Receiver Gain	30
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	3.0000
Acquisition Date	2017-05-08T11:50:09
Modification Date	2017-05-08T03:51:00
Spectrometer Frequency	369.72
Spectral Width	7183.9
Lowest Frequency	-793.5
Nucleus	1H
Acquired Size	21552
Spectral Size	65536

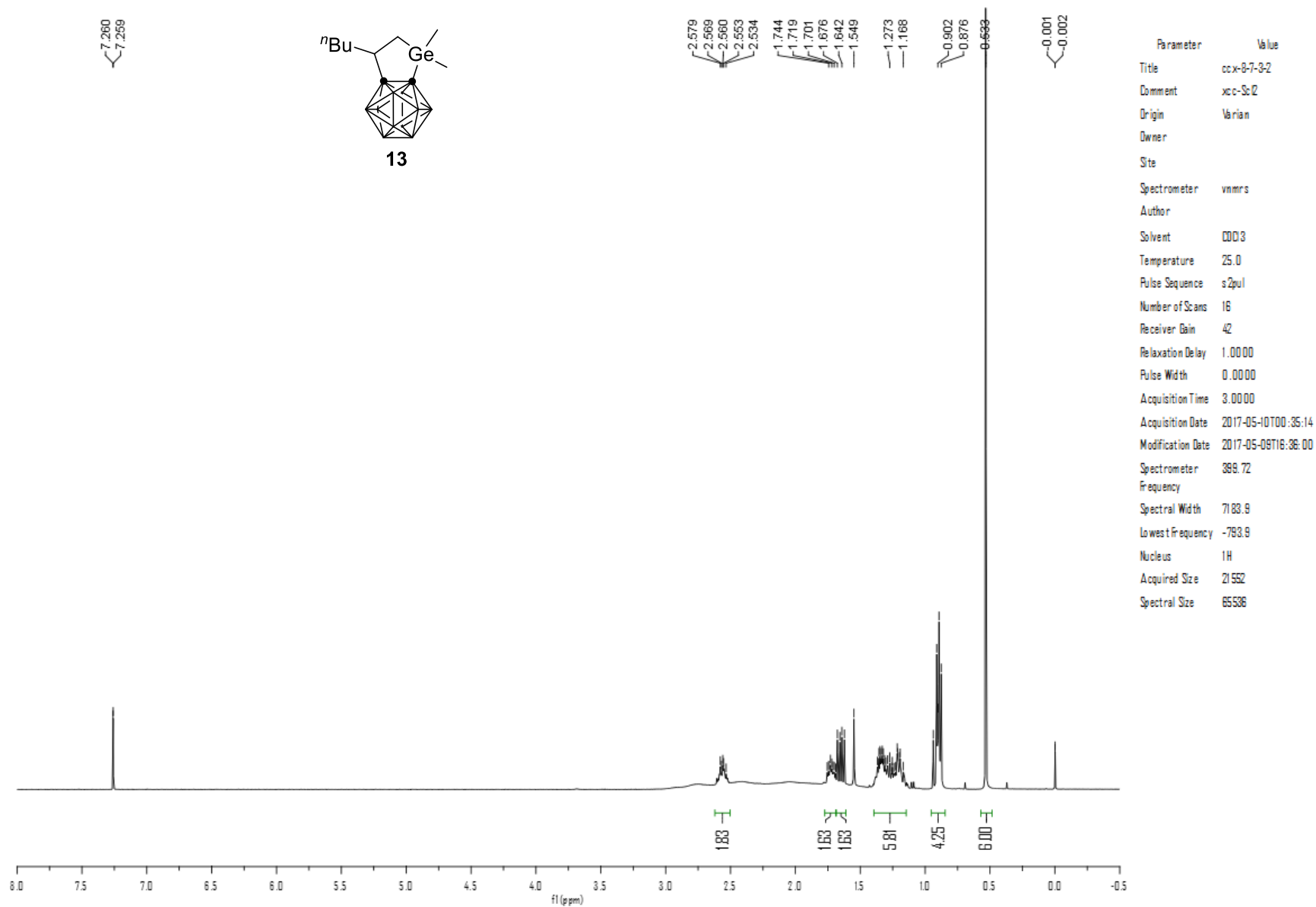


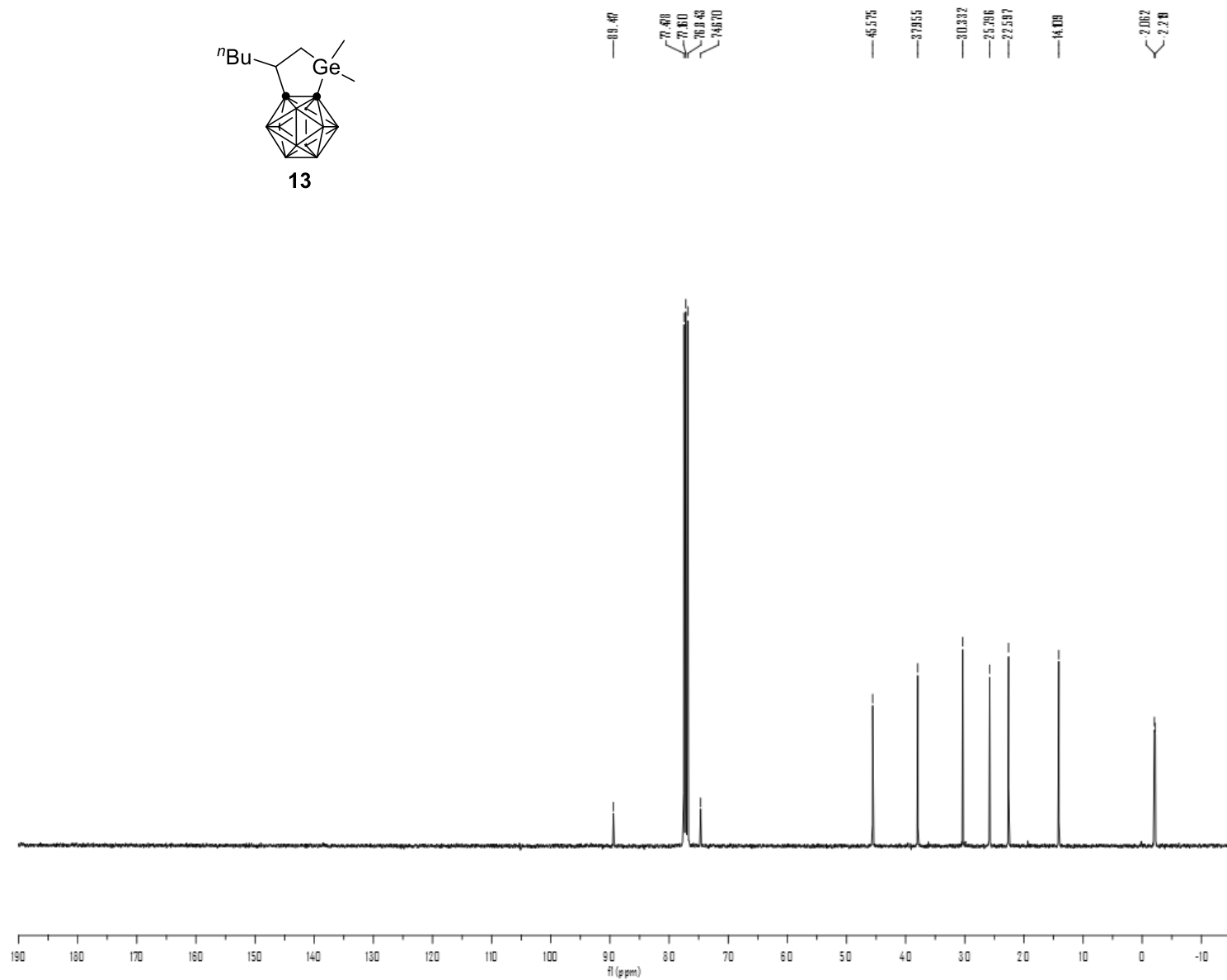
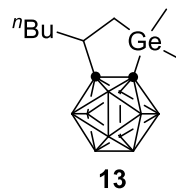


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-ccx-8-8-1/1/pdata/1/1r
Title	20120606-ccx-8-8-1
Comment	
Origin	UXNMR Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	30.0
Pulse Sequence	aring1gy
Number of Scans	115
Receiver Gain	203
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.3195
Acquisition Date	2017-05-08T21:51:51
Modification Date	2017-05-08T15:02:52
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-25865.1
Nucleus	11B
Acquired Size	16384
Spectral Size	32768

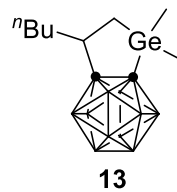


Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/2012060sn-ccx-8-8-1/2012060sn-ccx-8-8-1/pdata/1/1r
Title	2012060sn-ccx-8-8-1
Comment	
Origin	DNMR, Bruker Analytische Messtechnik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl_3
Temperature	30.0
Pulse Sequence	zgpg30
Number of Scans	184
Receiver Gain	11585
Relaxation Delay	1.0000
Pulse Width	4.0000
Acquisition Time	0.3277
Acquisition Date	2017-05-10T16:11:04
Modification Date	2017-05-10T09:12:22
Spectrometer Frequency	149.21
Spectral Width	10000.0
Lowest Frequency	-50103.8
Nucleus	
Acquired Size	32768
Spectral Size	32768

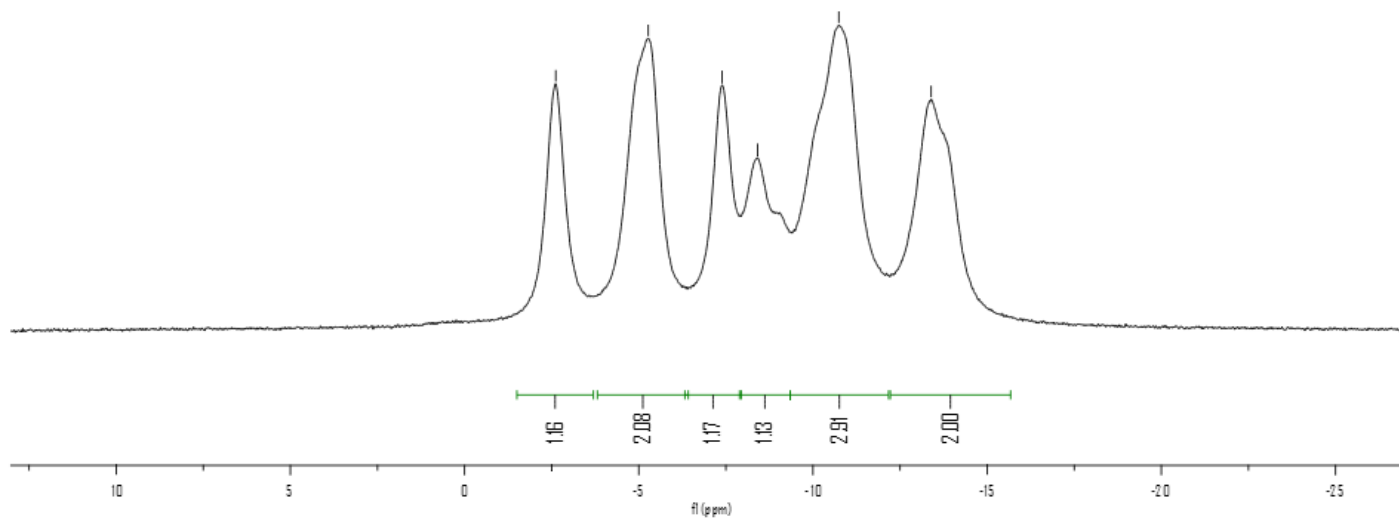




Parameter	Value
Title	ccx-8-7-9-2C
Comment	Std carbon
Origin	Varian
Owner	
Site	
Spectrometer	nmr5
Author	omcl
Solvent	cdcl3
Temperature	20.0
Pulse Sequence	s2pul
Number of Scans	10276
Receiver Gain	60
Relaxation Delay	1.0000
Pulse Width	0.0000
Acquisition Time	1.3005
Acquisition Date	2017-05-10T00:30:15
Modification Date	2017-05-09T23:05:00
Spectrometer Frequency	100.60
Spectral Width	24509.8
Lowest Frequency	-1676.3
Nucleus	13C
Acquired Size	31875
Spectral Size	65536



— 2.87
— 5.274
— 7.392
— 8.40
— 10.742
— 13.393



Parameter	Value
Data File Name	C:/Users/cuichunxiao/Desktop/20120606-ccx-8-7-2/1/ pdata/1/ 1r
Title	20120606-ccx-8-7-2
Comment	
Origin	UXNM R. Bruker Analytische Mess technik GmbH
Owner	root
Site	
Spectrometer	drx400
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	aring.1gy
Number of Scans	122
Receiver Gain	161
Relaxation Delay	0.0000
Pulse Width	5.0000
Acquisition Time	0.3195
Acquisition Date	2017-05-08T21:47:15
Modification Date	2017-05-08T15:03:02
Spectrometer Frequency	128.38
Spectral Width	51282.1
Lowest Frequency	-25995.1
Nucleus	1H
Acquired Size	16384
Spectral Size	32768