龙子湖新能源实验室

大型仪器设备技术验收报告

设 备 名 称 ：400MHz 固体核磁共振波谱仪

使 用 部 门 ：公共科学技术中心

验收负责人 ：李行

验 收 日 期 ：2024.11.30

龙子湖新能源实验室综合事务部

设备基本情况登记

设备名称		400MHz 固体核磁共振波谱仪		
规格型号		AVANCE NEO 400	数量	1
生产厂商		布鲁克	供应商	布鲁克（北京）科技有限公司
出厂日期		2024 年 8 月	设备经费来源	自筹
合同号		豫财单一采购-2023-134	到货日期	2024 年 8 月 16 日
安装使用地点		龙子湖新能源实验室 2 号楼北楼 123		
价格	人民币	6010000.00	外币	
使用责任人		李行	联系电话	18437911559

设备随机资料

序号	名称	份数	备注
1	超导磁体	1	
2	机柜	1	
3	$^{1}H/(^{15}N\text{-}^{31}P)$ 1.9mm 双共振固体探头	1	
4	$^{1}H/X/Y$ 4mm 三共振固体探头	1	
5	$^{1}H/(^{13}C\text{-}^{109}Ag)$ 7mm 双共振固体探头	1	
6	PC 工作站	1	
7	NMR 软件	1	
8	标准样品 1 套	1	
9	超导磁体用液氦真空输液管	1	

设备安装调试记录

记录人	李行	安装调试时间	2024.8.27

（安装、调试、运行过程及结果等记录、与厂商代表洽谈情况等）

2024年8月16日，由布鲁克（北京）科技有限公司运输到龙子湖新能源实验室2号楼北楼123房间，经验收，设备无损坏，设备数量与发货清单一致。

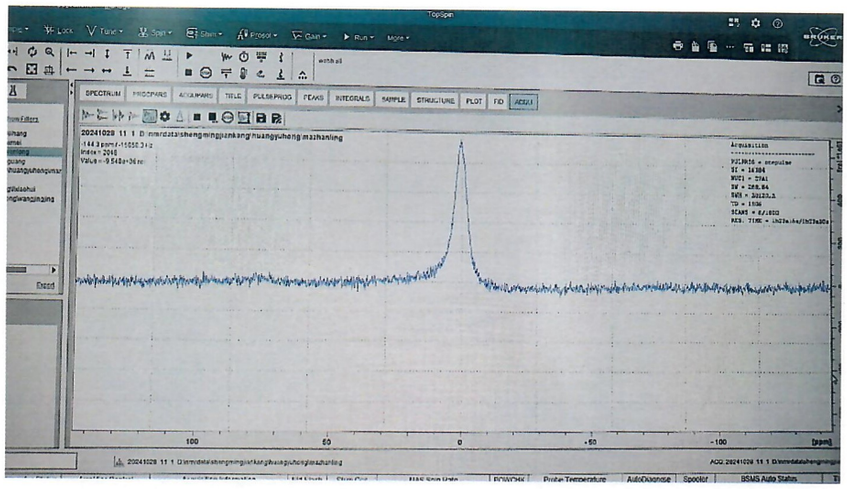
2024年8月27日，由布鲁克厂家委派方勇工程师对设备进行安装、调试。

1. 2024年8月27日 安装磁体；
2. 2024年8月28日至9月1日 安装磁体部件；
3. 2024年9月2日 往磁体液氦口加液氮，进行液氮预冷；
4. 2024年9月4日 往磁体液氦口加液氦；
5. 2024年9月5日 安装BST探头；
6. 2024年9月6日 安装工作站和信号放大器，进行调谐；
7. 2024年9月9日 磁体进行升场；
8. 2024年9月10日 低温匀场；
9. 2024年9月18日 安装氮气分离器；
10. 2024年9月19日 调试1.9mm、4mm和7mm探头。
11. 2024年9月25日至27日 进行固体核磁培训。
12. 经过一段时间的使用测试，设备运行正常。

结果：

设备及附件均已到货，设备已安装并进行基础培训。

数据结果显示：


TopSpin
SPECTRUM
PROCPARS
ACQUPARS
TITLE
PULSEPROG
PEAKS
INTEGRALS
SAMPLE
STRUCTURE
PLOT
FID
ACQU
100
50
0
-50
-100
[ppm]

设备验收记录

（仪器设备性能及技术指标与合同规定要求符合程度、验证方式方法、验证标准以及测试资料（包括曲线、图纸、照片等）并加以说明）

Installation Protocol - NMR Spectometer

NMR Probes

Description	Probe ID	Inspection Lot	Status
PH MASDVT400W1 BL4 X/Y/H	H8906_0110	2024-09-19	pass
PH MASDVT400W1 BL4 X/Y/H	H8906_0110	2024-09-19_TripleMode_HCN	pass
PH MASDVT400W1 BL4 X/Y/H	H8906_0110	2024-09-19_TripleMode_HPC	pass
PH MASDVT400W1 BL1.9 N-P/H	H171392_0003	2024-09-20	pass
PH MAS DVT 400W1 BL7 109Ag-Al/F-H	H132625_0012	2024-09-19	pass

Copies of all spectra (default and additional) are included in customer's PDF report.

Installation Checklist

Installation	pass	fail	n/a
All connections and grounding	☑	☐	☐
All firmware	☑	☐	☐
Cortab for required nuclei	☑	☐	☐
Lift / spin calibration	☑	☐	☐
Software licenses	☑	☐	☐
He / N2 log files activated	☑	☐	☐
MICS installed	☑	☐	☐
Remote monitoring enabled	☐	☐	☑
Customer agreed in activating AutoDiagnose	☐	☐	☑
AutoDiagnose successfully activated	☐	☐	☑
Customer agreed in installing LabScape Pro Care	☐	☐	☑
LabScape Pro Care successfully installed	☐	☐	☑

Customer Training	pass	fail	n/a
Basic safety	☑	☐	☐
Magnet safety and refilling	☑	☐	☐
Handling of cryogenic liquids	☑	☐	☐
Hardware overview	☑	☐	☐
Console on/off operation	☑	☐	☐
Basic operation	☑	☐	☐
Troubleshooting	☑	☐	☐
Backup (nmr_save, Images)	☑	☐	☐
Introduction to IconNMR	☐	☐	☑
Assure-SST / Performance check	☐	☐	☑
CryoProbe	☐	☐	☑
Handling / cleaning of probe	☐	☐	☑
He cylinder exchange	☐	☐	☑
He compressor cooling	☐	☐	☑
RF heating / power limits	☐	☐	☑
RF routing	☐	☐	☑

Acceptance and Warranty	pass	fail	n/a
Explaination of warranty	☑	☐	☐
Spectrometer documentation	☑	☐	☐
Customer support hotlines	☑	☐	☐

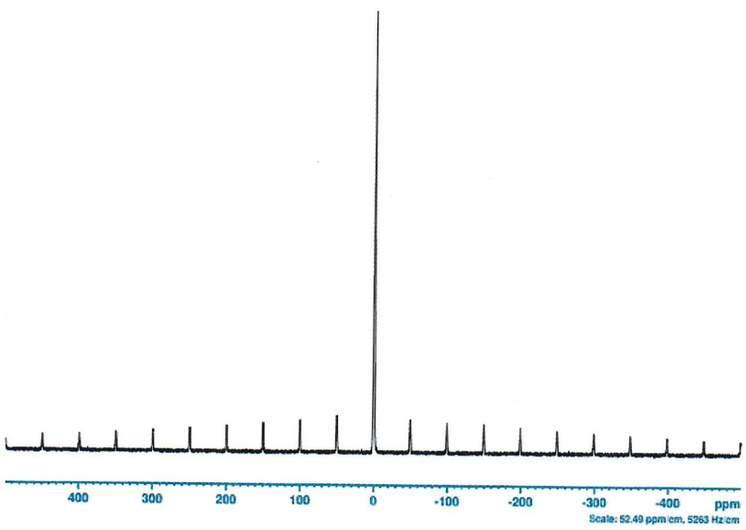
Optional Components	pass	fail	n/a
Sample Changer	☐	☐	☑
MAS controller	☑	☐	☐
High power equipment	☐	☐	☑
LC-NMR	☐	☐	☑
Liquid Handler SamplePro Tube	☐	☐	☑
Micro-Imaging	☐	☐	☑
Diffusion	☐	☐	☑
CryoProbe / Cryoplatform	☐	☐	☑
BNL / BSNL	☐	☐	☑
Additional cooling/heating units (like BCU1 / BCU2)	☐	☐	☑
LT-MAS (Low Temperature MAS equipment)	☐	☐	☑
Gyrotron magnet and DNP console	☐	☐	☑

ZFPT0008 Bruker BioSpin Report Name: 2024-09-24

实验结果：

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H8906_0110 PH MASDVT400W1 BL4 X/Y/H
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 5000 Hz)

Line width main [achieved/rated]: [142 <= 180] <pass>
Line width of side band number 8 (@ -40007 Hz) [achieved/rated]: [133 <= 200] <pass>

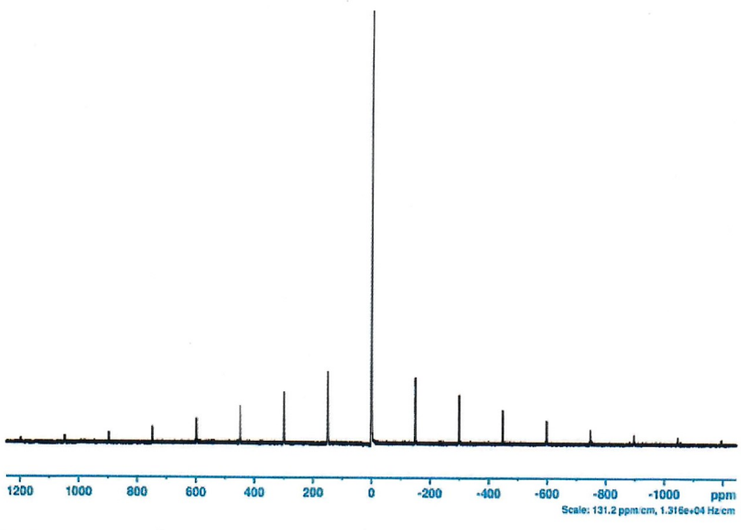


Bruker BioSpin

NPT_79Br_MAS_magicAngle

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H8906_0110 PH MASDVT400W1 BL4 X/Y/H
Sample: Potassium Bromide (KBr, 80 ul) (Z151220)
Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 15000 Hz)
Determination of spinning stability for 180 s
Pressure values in mbar: DrivePressure=1431/BearingPressure=3176/BearingSensePressure=3198/SupplyPressure=5886/SystemPressure=5325

Spin rate at maximum deviation [measured]: @ MASR 15000 Hz [15002 Hz]
Maximum deviation [achieved/rated]: @ MASR 15000 Hz [2 Hz <= 15 Hz] <pass>

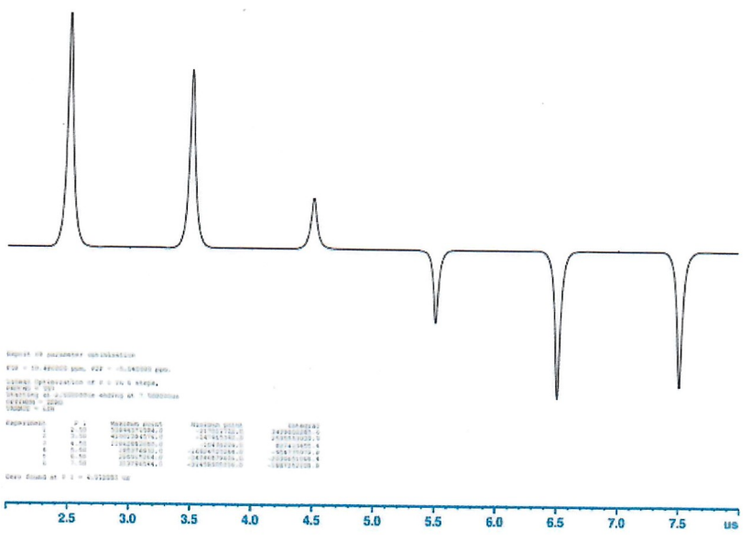


Bruker BioSpin

NPT_79Br_MAS_maxSpinRate

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H8906_0110 PH MASDVT400W1 BL4 X/Y/H
Sample: Adamantane (50 ul) (Z151221)
P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 15000 Hz)
ATTENTION: Updated PROSOL Tables with [2.50 us @ 87.0 W]

P90 MAS 1H pulse [achieved/rated]: @ 90.1 W [2.46 us <= 2.50 us] <pass>



Bruker BioSpin

NPT_1H_MAS_p90det_1h

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H8906_0110 PH MASDVT400W1 BL4 X/Y/H
Sample: Adamantane (50 ul) (Z151221)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 15000 Hz)

Bruker BioSpin

NPT_13C_MAS_sino_13c

+/NPT_shimfile_right.txt

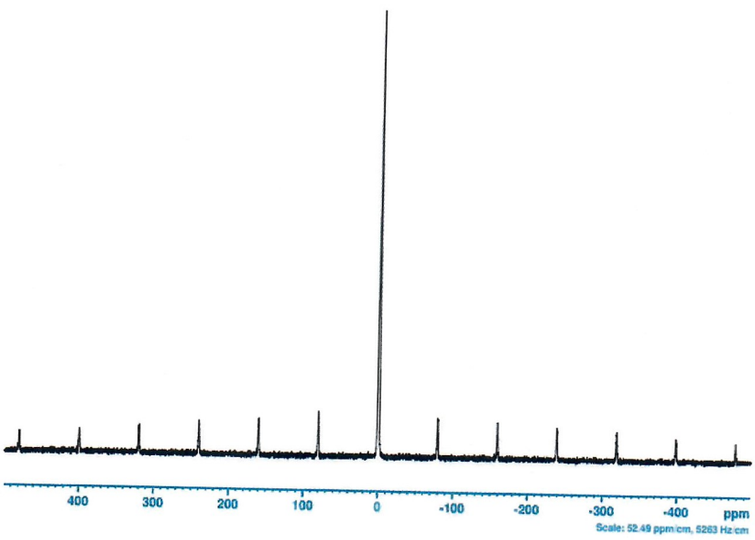
```
# Thu Sep 19 03:38:08 2024
#$$PROBEIDENTIFIER=H8906_0110
#$$PROBENAME=PH MASDVT400W1 BL4 X/Y/H
#$$MAGNETID=B2H0384070I02
#$$CRYOSTATID=D315-54-6922
#$$SHIMID=312532
#
# Active Shim Gradients
#
Z                       -17650
Z2                      0
Z3                      0
Z4                      0
Z5                      0
X                       0
XZ                      0
XZ2                     0
Y                       0
YZ                      0
YZ2                     0
XY                      0
XYZ                     0
(X2-Y2)                 -66000
(X2-Y2)Z                0
X3                      0
Y3                      0
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1]     -8560.25000000
SHIM_SETTING [ 2]         0.00000000
SHIM_SETTING [ 3]         0.00000000
SHIM_SETTING [ 4]         0.00000000
SHIM_SETTING [ 5]         0.00000000
SHIM_SETTING [ 6]         0.00000000
SHIM_SETTING [ 7]         0.00000000
SHIM_SETTING [ 8]         0.00000000
SHIM_SETTING [ 9]    -34716.00000000
SHIM_SETTING [10]         0.00000000
SHIM_SETTING [11]         0.00000000
SHIM_SETTING [12]         0.00000000
SHIM_SETTING [13]         0.00000000
SHIM_SETTING [14]      2741.90000052
SHIM_SETTING [15]     13394.48461080
SHIM_SETTING [16]         0.00000000
SHIM_SETTING [17]      1323.00000356
SHIM_SETTING [18]         0.00000000
SHIM_SETTING [19]         0.00000000
SHIM_SETTING [20]         0.00000000
```

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H171392_0003 PH MASDVT400W1 BL1.9 N-P/H
Sample: Potassium Bromide (KBr, 13.1 ul) (Z151260)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 8000 Hz)

Line width main [achieved/rated]: [133 <= 180] <pass>
Line width of side band number 5 (@ -40009 Hz) [achieved/rated]: [139 <= 200] <pass>

Bruker BioSpin

NPT_79Br_MAS_magicAngle

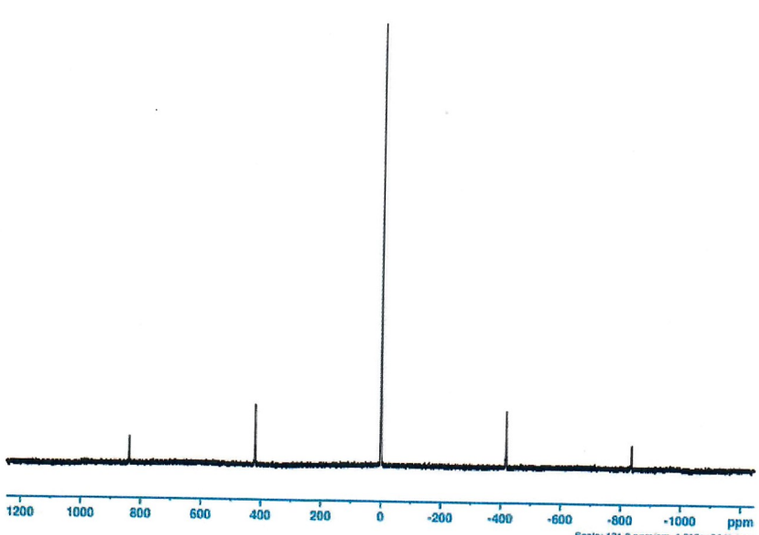


NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H171392_0003 PH MASDVT400W1 BL1.9 N-P/H
Sample: Potassium Bromide (KBr, 13.1 ul) (Z151260)
Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 42000 Hz)
Determination of spinning stability for 180 s
Pressure values in mbar: DrivePressure=3247/BearingPressure=3116/BearingSensePressure=3140/SupplyPressure=5776/SystemPressure=5236

Spin rate at maximum deviation [measured]: @ MASR 42000 Hz [41992 Hz]
Maximum deviation [achieved/rated]: @ MASR 42000 Hz [8 Hz <= 42 Hz] <pass>

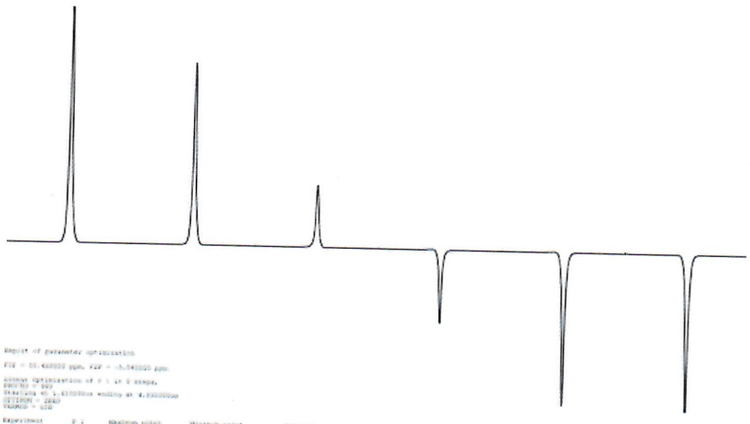
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate



NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H171392_0003 PH MASDVT400W1 BL1.9 N-P/H
Sample: Adamantane (13.1 ul) (Z151261)
P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 35000 Hz)
ATTENTION: Updated PROSOL Tables with [1.61 us @ 41.4 W].

P90 MAS 1H pulse [achieved/rated]: @ 42.1 W [1.60 us <= 1.61 us] <pass>



Bruker BioSpin

NPT_1H_MAS_p90det_1h

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H171392_0003 PH MASDVT400W1 BL1.9 N-P/H
Sample: Adamantane (13.1 ul) (Z151261)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 30000 Hz)

Bruker BioSpin

NPT_13C_MAS_sino_13c

*/NPT_shimfile_right.txt

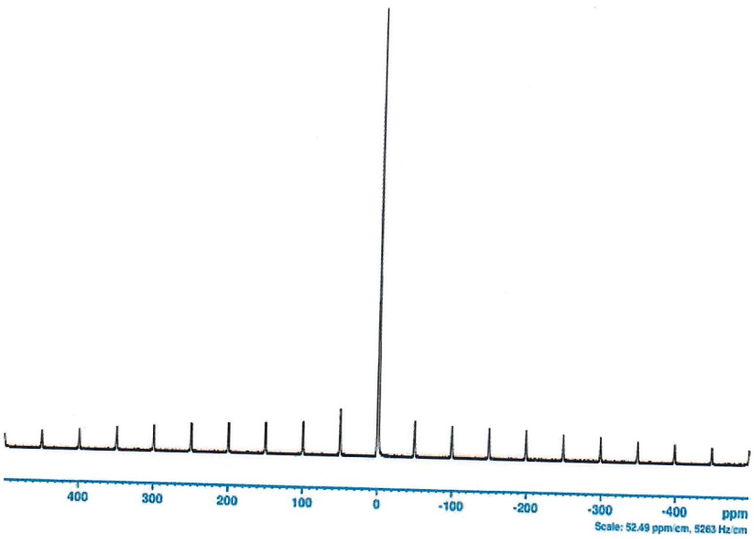
```
# Tue Sep 24 02:21:05 2024
##$$PROBEIDENTIFIER=H171392_0003
##$$PRONAME=PH MASDVT400W1 BL1.9 N-P/H
##$$MAGNETID=BZH03840702Z02
##$$CRYOSTATID=D315-54-6922
##$$SHIMID=312532
#
# Active Shim Gradients
#
Z                       -22600
Z2                      0
Z3                      0
Z4                      0
Z5                      0
X                       0
XZ                      0
XZ2                     0
Y                       0
YZ                      47600
YZ2                     0
XY                      0
XYZ                     0
(X2-Y2)                 -103500
(X2-Y2)Z                0
X3                      0
Y3                      0
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1]   -10961.00000000
SHIM_SETTING [ 2]        0.00000000
SHIM_SETTING [ 3]        0.00000000
SHIM_SETTING [ 4]        0.00000000
SHIM_SETTING [ 5]        0.00000000
SHIM_SETTING [ 6]        0.00000000
SHIM_SETTING [ 7]        0.00000000
SHIM_SETTING [ 8]        0.00000000
SHIM_SETTING [ 9]   -54441.00000000
SHIM_SETTING [10]        0.00000000
SHIM_SETTING [11]        0.00000000
SHIM_SETTING [12]    25037.60000000
SHIM_SETTING [13]        0.00000000
SHIM_SETTING [14]     2743.90000052
SHIM_SETTING [15]    13394.48461080
SHIM_SETTING [16]        0.00000000
SHIM_SETTING [17]     1323.00000356
SHIM_SETTING [18]        0.00000000
SHIM_SETTING [19]        0.00000000
SHIM_SETTING [20]        0.00000000
```

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H132625_0012 PH MAS DVT 400W1 BL7 109Ag-Al/F-H
Sample: Potassium Bromide (KBr, 234 ul) (Z151210)
Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle, spin rate 5000 Hz)

Line width main [achieved/rated]: [127 <= 180] <pass>
Line width of side band number 8 (@ -40005 Hz) [achieved/rated]: [124 <= 200] <pass>

Bruker BioSpin

NPT_79Br_MAS_magicAngle

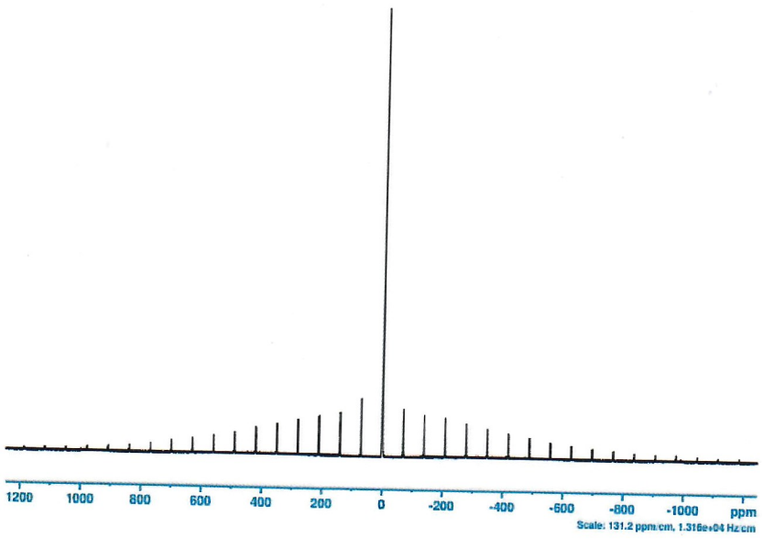


NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H132625_0012 PH MAS DVT 400W1 BL7 109Ag-Al/F-H
Sample: Potassium Bromide (KBr, 234 ul) (Z151210)
Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate, spin rate 7000 Hz)
Determination of spinning stability for 180 s
Pressure values in mbar: DrivePressure=1400/BearingPressure=3164/BearingSensePressure=3187/SupplyPressure=5825/SystemPressure=5269

Spin rate at maximum deviation [measured]: @ MASR 7000 Hz [6998 Hz]
Maximum deviation [achieved/rated]: @ MASR 7000 Hz [2 Hz <= 7 Hz] <pass>

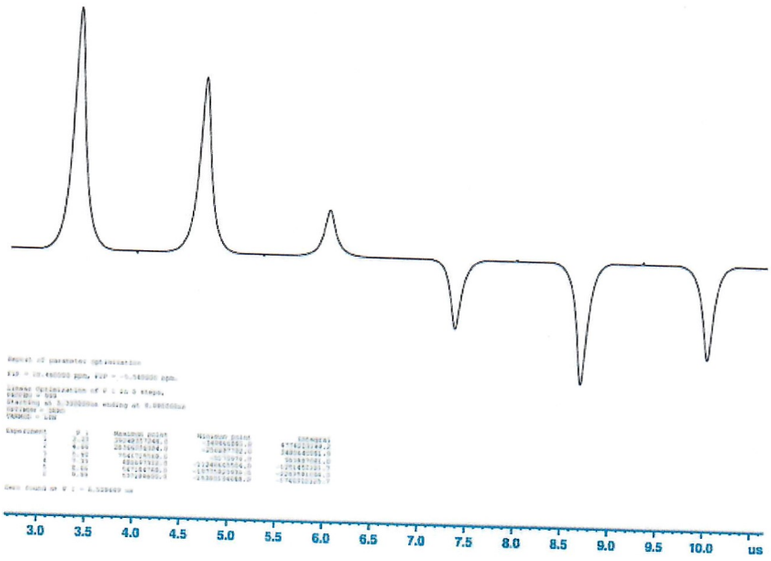
Bruker BioSpin

NPT_79Br_MAS_maxSpinRate



NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H132625_0012 PH MAS DVT 400W1 BL7 109Ag-Al/F-H
Sample: Adamantane (234 ul) (Z151211)
P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h, spin rate 7000 Hz)
ATTENTION: Updated PROSOL Tables with [3.33 us @ 204.4 W].

P90 MAS 1H pulse [achieved/rated]: @ 212.8 W [3.26 us <= 3.33 us] <pass>



Bruker BioSpin

NPT_1H_MAS_p90det_1h

NMR TEST ACCEPTANCE *** System: AV NEO (400.18 MHz) *** TopSpin 4.4.0
Probe: H132625_0012 PH MAS DVT 400W1 BL7 109Ag-Al/F-H
Sample: Adamantane (234 ul) (Z151211)
13C sensitivity, MAS (NPT_13C_MAS_sino_13c, spin rate 5000 Hz)

Bruker BioSpin

NPT_13C_MAS_sino_13c

+/NPT_shimfile_right.txt

```
# Thu Sep 19 10:22:34 2024
#$$PROBEIDENTIFIER=H132625_0012
#$$PROBENAME=PH MAS DVT 400W1 BL7 109Ag-Al/F-H
#$$MAGNETID=BZH03840701Z02
#$$CRYOSTATID=D315-54-6922
#$$SHIMID=312532
#
# Active Shim Gradients
#
Z                       -20650
Z2                      0
Z3                      0
Z4                      0
Z5                      0
X                       0
XZ                      0
XZ2                     0
Y                       0
YZ                      -22800
YZ2                     0
XY                      0
XYZ                     0
(X2-Y2)                 -60500
(X2-Y2)Z                0
X3                      0
Y3                      0
#
IEEE64_VERSION_CODE 1
#
# Shim currents
#
SHIM_SETTING [ 1]    -10015.25000000
SHIM_SETTING [ 2]         0.00000000
SHIM_SETTING [ 3]         0.00000000
SHIM_SETTING [ 4]         0.00000000
SHIM_SETTING [ 5]         0.00000000
SHIM_SETTING [ 6]         0.00000000
SHIM_SETTING [ 7]         0.00000000
SHIM_SETTING [ 8]         0.00000000
SHIM_SETTING [ 9]    -31823.00000000
SHIM_SETTING [10]         0.00000000
SHIM_SETTING [11]         0.00000000
SHIM_SETTING [12]    -11992.80000000
SHIM_SETTING [13]         0.00000000
SHIM_SETTING [14]      2741.90000052
SHIM_SETTING [15]     13394.48461080
SHIM_SETTING [16]         0.00000000
SHIM_SETTING [17]      1323.00000356
SHIM_SETTING [18]         0.00000000
SHIM_SETTING [19]         0.00000000
SHIM_SETTING [20]         0.00000000
```

设备验收小组意见

验收小组结论意见	同意验收 验收小组组长（签字） 宋玉婷 年 月 日

设备验收小组成员：

姓名	单位	签字
宋玉婷	龙子湖新能源实验室	宋玉婷
吕婉雪	龙子湖新能源实验室	吕婉雪
李申	龙子湖新能源实验室	李申
郑双双	龙子湖新能源实验室	郑双双
李行	龙子湖新能源实验室	李行