

Customer Information

Customer Name	Prof. Steven Brown
Operator Name	Dr Trent Franks
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Bruker Information

Office	Coventry
Engineer	Ariana Jones
Central Hotline Phone	0247 6855333
Central Hotline E-Mail	service.bbio.uk@bruker.com

Spectrometer Information

Order No.	408457
Contract No.	
System	Avance Neo 1000
Console Part and Serial No	HCAB-20 / 5
Coil	
Dewar	
Location	
TopSpin Version	TopSpin 4.0.9 - Build 597

Acceptance

I, an authorized customer representative, acknowledge that the above referenced system was installed and demonstrated to operate in accordance with the specifications mutually agreed upon by both parties. We accept the delivery and installation of this system as complete (except for items excluded below) and release Bruker from any further obligation, other than those obligations as specified during the warranty period. With this signature, the warranty period for non-excluded items commences according to the contractual agreement.

The warranty starts on Dec 22, 2020.

Place: Coventry, UK

Date: Dec 22, 2020

Place: Coventry, UK

Date: Dec 22, 2020

Prof. Steven Brown

Customer Representative Signature

Ariana Jones

Bruker Representative Signature

NMR Probe

Description	Probe ID	Inspection Lot	Status
PH MASDVT1000S6 BL1.9 X/H NO_/E	H170090_0001	1.9mm_HX_Install	pass

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

Installation Checklist

Installation	pass	fail	n/a	Optional Components	pass	fail	n/a
All connections and grounding	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Sample Changer	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
All firmware	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	MAS controller	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Cortab for required nuclei	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	High power equipment	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Lift / spin calibration	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	LC-NMR	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Software licenses	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Liquid Handler SamplePro Tube	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
He / N2 log files activated	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Micro-Imaging	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
MICS installed	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Diffusion	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
				CryoProbe / Cryoplatform	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Customer Training	pass	fail	n/a	BNL / BSNL	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Basic safety	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Additional cooling/heating units (like BCU1 / BCU2)	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Magnet safety and refilling	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	LT-MAS (Low Temperature MAS equipment)	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Handling of cryogenic liquids	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>	Gyrotron magnet and DNP console	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Hardware overview	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Console on/off operation	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Basic operation	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Troubleshooting	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Backup (nmr_save, Images)	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Introduction to IconNMR	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Assure-SST / Performance check	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
CryoProbe	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Handling / cleaning of probe	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
He cylinder exchange	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
He compressor cooling	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
RF heating / power limits	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
RF routing	<input type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>				
Acceptance and Warranty	pass	fail	n/a				
Explanation of warranty	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>				
Spectrometer documentation	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>				
Customer support hotlines	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>				

General Test Information

Summary of Inspection Lot

Description	Probe ID	Inspection Lot
PH MASDVT1000S6 BL1.9 X/H NO_I/E	H170090_0001	1.9mm_HX_Install

Experiments Measured

Sample	Experiment	Status
Z151260	Magic Angle setting, MAS (NPT_79Br_MAS_magicAngle)	pass
Z151260	Maximum spin rate testing, MAS (NPT_79Br_MAS_maxSpinRate)	pass
Z151260	Optimization of 79Br frequency (NPT_79Br_MAS_fieldsetting)	pass
Z151261	Optimization of 13C frequency (NPT_13C_MAS_fieldsetting_dec1h)	pass
Z151261	P90 1H pulse calibration, MAS (NPT_1H_MAS_p90det_1h)	pass
Z151260	P90 79Br pulse calibration, MAS (NPT_79Br_MAS_p90det_79br)	pass
Z151263	P90 13C 1H-13C CP pulse calibration, MAS (NPT_13C_MAS_p90det_cp1h_13c)	pass
Z151261	P90 13C pulse calibration, MAS (NPT_13C_MAS_p90det_13c)	pass
Z151263	P90 15N 1H-15N CP pulse calibration, MAS (NPT_15N_MAS_p90det_cp1h_15n)	pass
Z151264	P90 31P 1H-31P CP pulse calibration, MAS (NPT_31P_MAS_p90det_cp1h_31p)	pass
Z151262	CP 1H-13C sensitivity, MAS (NPT_13C_MAS_sino_cp1h_13c)	pass
Z151262	CP 1H-15N sensitivity, MAS (NPT_15N_MAS_sino_cp1h_15n)	pass
Z151264	CP 1H-31P sensitivity, MAS (NPT_31P_MAS_sino_cp1h_31p)	pass
Z151261	13C sensitivity, MAS (NPT_13C_MAS_sino_13c)	pass
Z151261	1H sensitivity, MAS (NPT_1H_MAS_sino_1h)	pass
Z151263	CP 1H-13C parameter optimization, MAS (NPT_13C_MAS_paropt_cp1h_13c)	pass
Z151263	CP 1H-15N parameter optimization, MAS (NPT_15N_MAS_paropt_cp1h_15n)	pass

Achieved Specifications

Pulse Width

Nucleus	Sample		90° Pulse		Power Limit [W]	Method	Status
			Duration [µs]	Power [W]			
1H	Z151261	spec.	2.00	-	150	direct	pass
		ach.	1.97	110.1			
13C	Z151261	spec.	3.50	-	200	direct	pass
		ach.	3.46	49.0			
13C	Z151263	spec.	3.50	-	200	with CP	pass
		ach.	3.49	47.9			
15N	Z151263	spec.	4.00	-	400	with CP	pass
		ach.	3.56	200.0			
31P	Z151264	spec.	4.00	-	250	with CP	pass
		ach.	3.17	225.6			
79Br	Z151260	spec.	5.00	-	200	direct	pass
		ach.	4.90	136.9			

Sensitivity

Nucleus	Sample		S/N	Remarks	Status
¹³ C	Z151262	spec.	-	sensitivity of ¹ H- ¹³ C cross-polarization	pass
		ach.	270.7		
¹⁵ N	Z151262	spec.	-	sensitivity of ¹ H- ¹⁵ N cross-polarization	pass
		ach.	34.0		
³¹ P	Z151264	spec.	-	sensitivity of ¹ H- ³¹ P cross-polarization	pass
		ach.	4595.8		

Sensitivity with NS

Nucleus	Sample		S/N	FWHM [Hz]	NS	Remarks	Status
¹ H	Z151261	spec.	-	-	-	noise: 20 ppm variable, method: sino best	pass
		ach.	12425.2	223.7	1		
¹³ C	Z151261	spec.	-	7.0	-	noise: 20 ppm variable, method: sino best	pass
		ach.	33.7	2.0	1		

Samples used for Inspection Lot

Sample	Description
Z151260	Potassium Bromide (KBr, 13.1 ul)
Z151261	Adamantane (13.1 ul)
Z151262	α -crystalline Glycine (10 mg, 13.1 ul)
Z151263	2- ¹³ C, ¹⁵ N alpha-glycine (10 mg, 13.1 ul)
Z151264	Ammonium Dihydrogenphosphate (NH ₄ H ₂ PO ₄ , 13.1 ul)

Remarks / Exclusions