Quantum-I*Plus* NMR Spectrometer

Product Manual

WMR/3-YF/P-C/SM/A1

Q.One Instruments Ltd.

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Quantum-I^{Plus} NMR Spectrometer Product Manual

Version: A1

No.: WMR/3-YF/P-C/SM/A1

Supporting documents:

SpinStudioJ User Manual (WMR/3-YF/P-C/YHCZ/B0)

SpinStudioJ Command and Parameter Manual (WMR/3-YF/P-C/MLCS/B0)

Installation Preparation Instructions for Quantum-I^{Plus} NMR Spectrometer (WMR/3-YF/P-C/ZB/C0)

Quantum NMR Spectrometer Healthy and Safety Notice(WMR/3-YF/P-C/JA/A0)

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Modification history:

A0: 2020.3, initial version.

A1: 2022.1, Add spectrometer components and connections diagram.

Q.One Instruments Ltd. reserves the right to change the technical specifications. The contents of this specification may be updated without informing the customer.

WMR, Q.One Inst, Q.One is the abbreviation of Q.One Instruments Ltd.

WNMR, BIXI and Quantum are the model codes of NMR spectrometer products of Q.One Instruments Ltd. WNMR-I, BIXI-I and Quantum-I refer to the same products.

Technical Support and Services

Service concept

Your satisfaction is our greatest success!

Scope of Service

1) Installation and maintenance of NMR spectrometer.
2) Customization of NMR Spectrometer.
3) User training (experimental operation, strong field safety, high-order nuclear magnetic resonance, etc.).
4) Spectrometer calibration and maintenance services during the life cycle of NMR spectrometer.
5) During the life cycle of NMR spectrometer, the following free services are provided:
   - SpinSdudioJ, the control and data processing software, is upgraded free of charge.
   - Major defects or major safety defects of the functions agreed in the contract shall be handled free of charge.

Please help us do better!

We are committed to providing excellent NMR spectrometers to continuously meet your current and future needs in using NMR spectrometers. Your feedback is very important to us. If you find any problems with spectrometer, software or manuals, or have any suggestions for improvement, please feel free to contact us.

Product consultation, sales, repair and technical support

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Service Commitment

Q.One Instruments Ltd.(Q.One) guarantees that if this product has defects such as failure and damage during the warranty period, Q.One will repair or replace the defective product or parts without charging for components and labor costs. Spectrometer components provided by yourself or purchased by Q.One are not covered by the warranty. Q.One's replacement components, modules and products are brand new. All replaced parts, modules and products will become the property of Q.One.

In order to obtain the services promised in this warranty statement, you shall notify Q.One of the defects during the warranty period and make appropriate arrangements for the performance of the services.

This warranty statement does not apply to any defect, failure or damage caused by improper use, improper maintenance or insufficient maintenance. Q.One is not obliged to provide the following services under this warranty statement: (1) Repair damages caused by disassembly, installation, repair or maintenance of products by non-Q.One service representatives. (2) Repair damages caused by improper use or connection with incompatible equipment. (3) Repair any damage or failure caused by the use of equipment not provided or specified by Q.One. (4) Repair products that have been changed or integrated with other products.

This warranty is made by Q.One regarding this product and is used to replace of any other express or implied warranty. Q.One refuses to give any implied warranty as to the suitability of this product for special purposes. For breach of this warranty, Q.One is responsible for repairing or replacing the defective products, which is the only remedy provided to you. Q.One is not responsible for any indirect or accidental damage to the products regardless of whether Q.One has been notified in advance of the possibility of such damage.

Security Summary

All manuals of Quantum series NMR spectrometer products use the following warning or prompt icons:

Warning: this icon is used to prompt you to strictly adhere to these rules. For breach of these principles, it may result in personal injury or death, or significant property damage.

Note: this icon is used to prompt you for these considerations, and failure to comply with these prompts may result in device damage or loss of data.


Prompt: this icon is used to indicate information you can refer to.

Warning

The following provisions must be complied with during the use and maintenance of the spectrometer. Q.One will not be responsible for any losses caused by non-compliance with the following warning provisions or intentional violation of the safety guidelines for the use of the spectrometer.

Persons implanted with medical equipment (such as artificial limbs, implanted cardiac pacemakers, etc.) are prohibited from entering the 5 Gauss line of the magnet.

The strong magnetic field of superconducting magnets will affect the normal operation of cardiac pacemakers and damage the artificial limbs or other metal implants worn.

Cardiac pacemaker carriers should consult cardiac pacemaker manufacturers and doctors to determine the impact of magnetic field on cardiac pacemakers or possible health risks. Other metal implant carriers should also confirm whether there is a risk.

Ferromagnetic metal articles are prohibited from entering the 10 Gauss line of the magnet.

The strong magnetic field around the magnet has strong attraction to articles containing steel, iron or other ferromagnetic materials, such as common tools, equipment, gas tanks, metal chairs, carts, etc. If these objects are not reliably fixed, they will fly to the magnet. The light ones will seriously affect the uniformity of the magnetic field, and the heavy ones will cause serious damage to the probe, Dewar and superconducting coil, and may cause personal injury. The greater the mass of an object, the greater the attraction of the magnet to it.

Only non-ferromagnetic articles (such as plastic, aluminum, wood, non-ferromagnetic metal, etc.) can be used around the magnet.

If the article is sucked to the magnet surface and cannot be removed manually, please contact Q.One.

After the magnet is installed, the marked Gaussian line range should be carefully checked.

WARNING Only Q.One authorized personnel are allowed to open the spectrometer package or casing, or make internal adjustments to the spectrometer.

There is a fatal high voltage inside the equipment. Please turn off the main power switch of PDU at the lower right foot at the rear of the cabinet before working inside the cabinet.

WARNING It is forbidden to replace or repair spectrometer components without authorization.

Unauthorized maintenance of spectrometer will cause personal injury or equipment damage, and unconditionally terminate the quality assurance agreement and contract service terms. Only Q.One service representatives are allowed to make changes to the Quantum-I Plus NMR spectrometer. If additional equipment needs to be installed or the spectrometer needs to be modified, please contact Q.One.

WARNING It is forbidden to work in an environment where flammable or toxic gases exist.

Working in an environment with flammable or toxic gases may cause explosion, fire or poisoning.

WARNING If the magnet is quenched, please leave the site immediately.

If the magnet quenches (the magnetic field suddenly disappears and a large amount of gas suddenly ejects from the top of the magnet), please leave the scene immediately. The sudden release of helium and nitrogen will cause rapid hypoxia in a certain area, thus possibly causing suffocation. Do not return to the site until the oxygen level returns to normal.

WARNING Prevent liquid helium or nitrogen from contacting any part of the body

The injury caused by liquid helium or liquid nitrogen in contact with the body is the same as that caused by burns. It is forbidden to place the head above the helium tube and nitrogen tube outlet above the magnet. Please seek medical treatment immediately when liquid nitrogen or liquid helium comes into contact with the body-especially when skin blisters or eyes are affected.

Filling the magnet with liquid nitrogen and liquid helium must be carried out by trained and experienced professionals.

WARNING Do not look inward from top of the upper tube

Unless the probe and sample tube have been removed, it is forbidden to look inward from the top of the upper tube. When the sample tube ejects from the probe, it may poke the eyes.

WARNING During temperature control experiments, it is forbidden to set the temperature beyond the boiling point and freezing point of the sample under the current air pressure.

When the temperature changes, the sample tube will bear too much pressure, which

may cause the sample tube to burst, and splashing glass and toxic substances will also cause injuries to the spectrometer or personnel. Before doing the temperature control experiment, please confirm the boiling point and freezing point of the sample under the current air pressure.

WARNING **Anti-impact magnet**

The center of gravity of the magnet is relatively high, so it may roll over after an earthquake or being hit by other heavy objects, causing injuries to personnel and causing the magnet to lose excess.

WARNING **Do not remove one-way valves on liquid nitrogen and liquid helium exhaust pipes**

The function of one-way valve is to prevent air from entering nitrogen and helium pipes. Moisture in the air will freeze after entering the magnet, causing air pipe blockage and oxygen liquefaction, which may bring safety risks. Except for filling liquid helium or liquid nitrogen, ensure that the check valve has been tightened reliably for the rest of the time.

Attention

The following terms and conditions must be complied with during the use and maintenance of the spectrometer. Q.One will not be responsible for any losses caused by non-compliance with the following precautions or intentional violation of the complete guidelines for the use of the spectrometer.

Magnetic media, such as bank cards, credit cards, watches, mobile phones, etc., are prohibited from entering the 5 Gauss line of the magnet.

The strong magnetic field around superconducting magnets will eliminate the magnetism of magnetic media, such as magnetic tapes, floppy disks, bank cards, etc., and watches will also be affected by the strong magnetic field.

Please carefully observe the 5 Gauss line range marked around the magnet.

Place the computer (including NMR workstation) outside the 5 Gauss line range of the magnet.

The hard disk of the computer may degauss and lead to data loss. Keep the computer (including NMR workstation) away from the magnet to prevent data loss or device damage.

Please check and record the liquid helium and liquid nitrogen level meters every day.

Record the readings of the level meter every day, and take the average value of the readings as the normal working flow value. At different atmospheric pressures, the readings of the level meter will vary slightly. If the volatile level meter reading suddenly

changes, please contact Q.One immediately. If the cause of abnormal reading cannot be eliminated, the magnet may be damaged.

CAUTION Take effective anti-static measures to avoid damage to electrostatic sensitive parts of the product.

The static electricity of human body will damage the system components, define the static electricity protection operation specification in the test process, effectively control the generation and discharge of static electricity, reduce the hidden trouble of static electricity, ensure the normal working state of the product,

1. NMR Spectrometer Laboratory Working Environment Management Requirements.
    1) NMR laboratories should hang warning signs at obvious places.
    2) The environment requires a temperature of 15-30 ℃ and a relative humidity of 50-60% in the laboratory. Equipped with a temperature and humidity meter, confirmed twice a day and recorded in the "Temperature and Humidity Record Table", take corresponding measures to make it meet the requirements in case of discrepancy.
    3) NMR laboratory requires electrostatic protection grounding. The working area has antistatic wrist and antistatic rubber.
2. Personnel Electrostatic Requirements:
    1) Test laboratory personnel, technical personnel and other relevant personnel related to the laboratory shall be trained before taking up their posts.
    2) All personnel entering the laboratory must wear effective anti-static work clothes, shoes and caps, and touch the human electrostatic releaser at the entrance to relieve the accumulated static electricity of the human body.
    3) All personnel must be equipped with anti-static wrist with rope when contacting the control cabinet, and ensure effective grounding.

3. Electrostatic Requirements for NMR Spectrometers:

   1) All kinds of equipment, tools, tooling and spectrometers in the working area of NMR spectrometer shall take electrostatic protection measures.

   2) The floor and workbench in the test work area shall be paved with antistatic rubber, and at least one grounding port shall be ensured every 5 meters to ensure effective grounding in daily use.

   3) The shell of NMR spectrometer shall be hard grounded (the grounded wire is the earth wire).

   4) ESD materials shall be selected for the material table, turnover box and packaging bag required for test.

Requirements for Posting Strong Magnetic Field Warning Signs

In order to warn of the existence and risks of strong magnetic field, users are obliged to post obvious signs of strong magnetic field damage, including measuring stray magnetic field with Gaussian meter.

Radio frequency radiation may also cause personal injury. Although Quantum series NMR spectrometer products have taken strict protective measures and passed necessary tests, it is still necessary for you to post radio frequency radiation risk warning signs.

Warning flag

Q.One provides a certain number of warning signs and warning tapes to help you realize your posting responsibilities. Signs must be posted before the magnet is lifted and meet the following requirements:

(1) Post a 10 Gauss warning sign along the horizontal and vertical 10 Gauss lines of the magnetic field to ensure that anyone attempting to enter the 10 Gauss line range can see the sign. It should be noted that signs should also be posted in the next room or on the adjacent floor. If the 10 Gauss magnetic field does not exceed 30cm through the fixed wall surface, or does not exceed 61cm above the magnet, no additional signs need to be posted.

(2) Post a 5 Gauss warning sign along the 5 Gauss line of the magnetic field to ensure that anyone attempting to enter the 5 Gauss line can see the sign. It should be noted that signs should also be posted in the next room or on the adjacent floor.

(3) Post strong magnetic field area hazard signs at each entrance to the magnetic field area to ensure that each sign should be outside the range of 5 gauss.

Note that if two or more magnetic fields overlap each other, or if the magnetic fields pass through large ferromagnetic objects (such as iron gates, metal beams, etc.), the range of stray

fields will exceed the calibrated range. In this case, you should use a Gaussian meter to measure the actual range of arrival of the 5 Gaussian magnetic field and the 10 Gaussian magnetic field.

If you need additional logos, please ask Q.One for them.

Public Activity Area

In addition to posting signs, Q.One strongly requires you to close or restrict public areas containing magnetic fields of 5 gauss or higher, which may include halls, corridors, etc.

Safety training

You must train anyone who may be exposed to a magnetic field of 5 Gauss or higher about magnetic field risks.

Radio frequency radiation suppression

The enclosure of the spectrometer system forms a shielding network for radio frequency radiation. Removing any part of the enclosure or modifying the internal equipment may cause greater radio frequency interference to the internal equipment of the system or increase the external radio frequency radiation of the system. Spectrometer operators have the responsibility to maintain the equipment in a state that meets the requirements of radio frequency radiation.

Contents

Preface

This manual introduces the principle, structure, use and maintenance methods of Quantum-I^{Plus} NMR spectrometer system, including introduction, installation, preparation, operation methods, system maintenance, common faults and treatment methods of Quantum-I Plus NMR spectrometer.

The contents of this manual are arranged as follows:

- Chapter 1: Quantum-I ^{Plus} NMR spectrometer, introducing the components and functions of the system.
- Chapter 2: Installation, introducing the installation preparation, receipt and transfer precautions of the system, as well as the installation methods of hardware and software, etc.
- Chapter 3: Preparation for use, introducing the startup of the system, inspection of working status and manual control, etc.
- Chapter 4: Usage methods, including how to prepare samples and how to conduct NMR experiments, etc.
- Chapter 5: Requirements for Use and Maintenance, introducing matters needing attention in the process of use and maintenance of the system.
- Chapter 6: Faults and Treatment, introduces the inspection and treatment methods of common simple faults in the system.

Please refer to the following documents for how to use SpinSdudioJ software:

1) SpinStudioJ User Manual.

2) SpinStudioJ Command and Parameter Manual.

3) SpinStudioJ NMR Experiment Quick Reference Manual.

Document Format

All manuals of the Quantum-I NMR spectrometer are marked in the following special format:

- The content of the regular script is prompt or warning, they also use ICONS 

、  to mark.
- *Italics* indicates other file names introduced in this manual, such as: *"please refer to SpinSdudioJ User Manual"*.
- ***Bold italic*** indicates the command that can be typed in the command line of SpinStudio software, such as: "execute command "***go***" to acquire FID data".

Other manuals

Other manuals accompanying this manual include:

- Installation preparation instructions for Quantum-I Plus NMR spectrometer. No.: WMR/3-YF-YJ/P-B/AZ/A0.
- SpinStudioJ User Manual. No.: WMR/3-YF/P-C/YHCZ/B0.
- SpinStudioJ Command and Parameter Manual. No.: WMR/3-YF/P-C/MLCS/B0.

The "Quantum-I Plus NMR Spectrometer Installation Preparation Manual" will be sent to you after you have ordered the Quantum-I Plus NMR Spectrometer to guide you in the preparation of the installation site and facilities. The "Quantum-I Plus NMR Spectrometer Installation Preparation Manual" contains the "Quantum-I Plus NMR Spectrometer Installation Condition Confirmation" to confirm the preparation work. The rest manuals will be sent to you along with the Quantum NMR spectrometer system. In the process of using Quantum-I Plus NMR spectrometer, you can refer to the manuals provided by Q.One and use SpinStudioJ to carry out NMR experiments to complete the daily maintenance and maintenance of the spectrometer.

Quantum-I Plus NMR Spectrometer

Product Manual

1 Quantum-I Plus NMR Spectrometer

1.1 Introduction to the System

Quantum-I Plus NMR Spectrometer is a modern independent large-scale scientific spectrometer produced by Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, which integrates the research and development achievements of the top domestic technical teams and the latest technological development achievements in the world. Q.One Instruments Ltd. is a manufacturer of Quantum-I Plus NMR Spectrometer. We are committed to providing excellent NMR spectrometers to continuously meet your current and future needs in using NMR spectrometers. Our strong scientific research and technical strength and localized technical support team provide a solid guarantee for you to use, maintain, upgrade or customize NMR spectrometer.

Quantum-I Plus NMR Spectrometer is designed for liquid and solid nuclear magnetic resonance applications. The standard system configuration meets the basic needs of most users, but at the same time it also allows customers to put forward specialized functional customization requirements for the system according to their own needs. In addition to the upgrade service promised by Q.One, customers can also put forward new upgrade or modification requirements during the use of the system.

1.2 Working principle

1.2.1 Nuclear Magnetic Resonance(NMR) Principle

In 1946, E. M. Purcell and F. Bloch independently discovered the nuclear magnetic resonance (NMR) phenomenon of matter in general state by different methods. The so-called nuclear magnetic resonance refers to the resonance phenomenon of nuclei with non-zero spin quantum number. In the static magnetic field B0, a set of split energy levels are formed due to the interaction between magnetic moment and magnetic field, and the nuclei are irradiated

with external electromagnetic waves. When the frequency of electromagnetic waves is equal to the frequency of nucleus Lamo precession angle, the resonance phenomenon occurs due to transition between nucleus energy levels.

There is a strict relationship between the angular frequency of the electromagnetic wave irradiating the nucleus and the static magnetic field B0:

$$\omega = \gamma B_0$$

Where:

$\omega = 2\pi f_0$ f_0 -Electromagnetic wave angular frequency or nuclear Lamo precession angular frequency, which is the electromagnetic wave frequency in Hz.

γ -The gyromagnetic ratio of the nucleus is the natural attribute of the nucleus, and the gyromagnetic ratio of each nucleus is a different constant.

B0-Static magnetic field strength in Tesla T.

1.2.2 NMR Spectrometer

Spectrometers developed by using the principle of nuclear magnetic resonance to observe the structure, composition or molecular dynamics of nuclei or to realize application by using the characteristics of nuclei are collectively referred to as nuclear magnetic resonance spectrometers.

According to the requirements of various applications, Various NMR spectrometers have been developed, Such as nuclear magnetic resonance spectrometer, nuclear magnetic resonance imaging instrument, nuclear magnetic resonance logging instrument, nuclear magnetic resonance water exploration instrument, nuclear magnetic resonance analyzer, nuclear magnetic resonance surface detector, nuclear magnetic resonance magnetic field meter and field meter, etc., nuclear magnetic resonance spectrometer has become a very important spectrometer equipment to solve major scientific, economic, environmental and social problems.

Quantum-I Plus NMR spectrometer is a nuclear magnetic resonance spectrometer, which is a high-resolution nuclear magnetic resonance spectrometer used to measure the nuclear

magnetic resonance spectrum and related parameters of one or more nuclei in a substance and to analyze the fine structure of compound molecules.

1.2.3 Chemical shift

Under the same intensity of external magnetic field B0, the rotating magnetic ratio of different nuclei is different, so the resonance frequency of different nuclei is different. This is the fundamental basis for nuclear magnetic resonance spectrometer to measure various nuclei with different radio frequency frequencies.

Due to the different chemical environment in which the same nucleus is located, under the same external magnetic field B0, the actual magnetic field strength borne by the nucleus is also different:

$$B_{nuc} = B_0(1-\sigma)$$
$$\omega_{nuc} = \gamma(1-\sigma)B_0$$

Where:

σ - Shielding constant, numerical range $10^{-3\sim-5}$.

B_{nuc}-the actual magnetic field strength in which the nucleus is located.

ω_{nuc}-The actual resonance angular frequency of nuclear magnetism.

The change of resonance frequency of the observed nucleus due to the change of chemical environment is expressed by the relative chemical shift value. Chemical shift is the basis for nuclear magnetic resonance spectrometer to measure and distinguish various chemical substances.

Many characteristics of NMR spectral lines, such as chemical shift, spectral splitting, spectral line width, shape, relaxation time T1/T2, etc., can quickly, accurately and with high resolution determine various molecular structures by analyzing the characteristics of NMR spectral lines without damaging the sample structure.

In order to simultaneously excite the resonance signals of nuclei in the same substance in various chemical environments (similar but different resonance frequencies), Modern nuclear magnetic resonance spectrometers all use radio frequency pulses to excite. The transmitter

emits one or a series of narrow radio frequency pulses while exciting the resonance of observed nuclei with different chemical shift values in a small frequency range near the radio frequency center.

1.3 Application Scope of NMR Spectrometer

Nuclear magnetic resonance spectrometer is an important spectroscopic research method to study the composition, molecular structure and dynamics of substances. Nuclear magnetic resonance spectroscopy can be used to characterize solid, liquid, liquid crystal and amorphous substances, as well as pure and mixed substances. It can be widely used in the research and development of physics, chemistry, chemical industry, materials, biology, medicine, pharmacy, drug detection, proteomics, metabolomics, high-yield breeding, food processing and other fields, and has become a very important spectrometer equipment to solve major scientific, economic, environmental and social problems.

Nuclear magnetic resonance spectrometers are commonly used in laboratories of universities, research institutions, enterprises, inspection institutions and other units, and are placed in special laboratory rooms, and are supervised and operated by special personnel for students, teachers, research and development personnel, testing personnel and so on.

CAUTION *This product is a testing equipment. Q.One is only responsible for the true validity of the data. The source and processing of the tested samples, the processing and use of the collected data, and the economic and legal risks arising therefrom shall be borne by the users themselves.*

CAUTION *This product is non-medical equipment and is forbidden to be used clinically in hospitals. The economic and legal risks brought about by research and tests for medical purposes shall be borne by users themselves.*

1.4 Spectrometer Introduction

1.4.1 Spectrometer Components

The spectrometer component configuration of the standard Quantum-I Plus NMR spectrometer for routine test requirements is shown in the following table. Q.One also supports customized configuration requirements for users' special needs.

Table 1 Quantum-I Plus NMR Spectrometer Configuration

Part Name	Standard Configuration	Expansion Capability
Pulse transmitter	2 channels	3 channels
Digital receiver	1 channel	2 channels
D-lock system	1	D/F Lock
Pulse gradient	10A,1 channel	20A, 1 channel
RT shimming system	23 channels	40 channels
Superconducting magnet	400MHz, 600MHz	200MHz, 300MHz, 500MHz
Sample tube diameter	5mm	3mm, 10mm
Automatic injector	24 sample	60 samples

Fig. 1 Quantum-I Plus NMR Spectrometer Parts

The standard configuration of the Quantum-I Plus NMR spectrometer includes the following features, as shown in Figure 1:

1) Console Cabinet: including main control system (CCS, Console Control System), RF power amplifier and Magnetic Field Control System (MFCS, Magnetic Field Control

System).

2) Preamplifier System: includes a transceiver switch and a preamplifier for each of proton, X nuclear and D/F lock.
3) Magnet: includes superconducting magnet, sample injection tube, probe, room temperature shim coil and other supporting components.
4) NMR Workstation: includes a standard computer and Q.One NMR spectrometer control and data processing software SpinStudioJ.

Connections between each components of the Quantum-I Plus NMR spectrometer was shown in Figure 2.

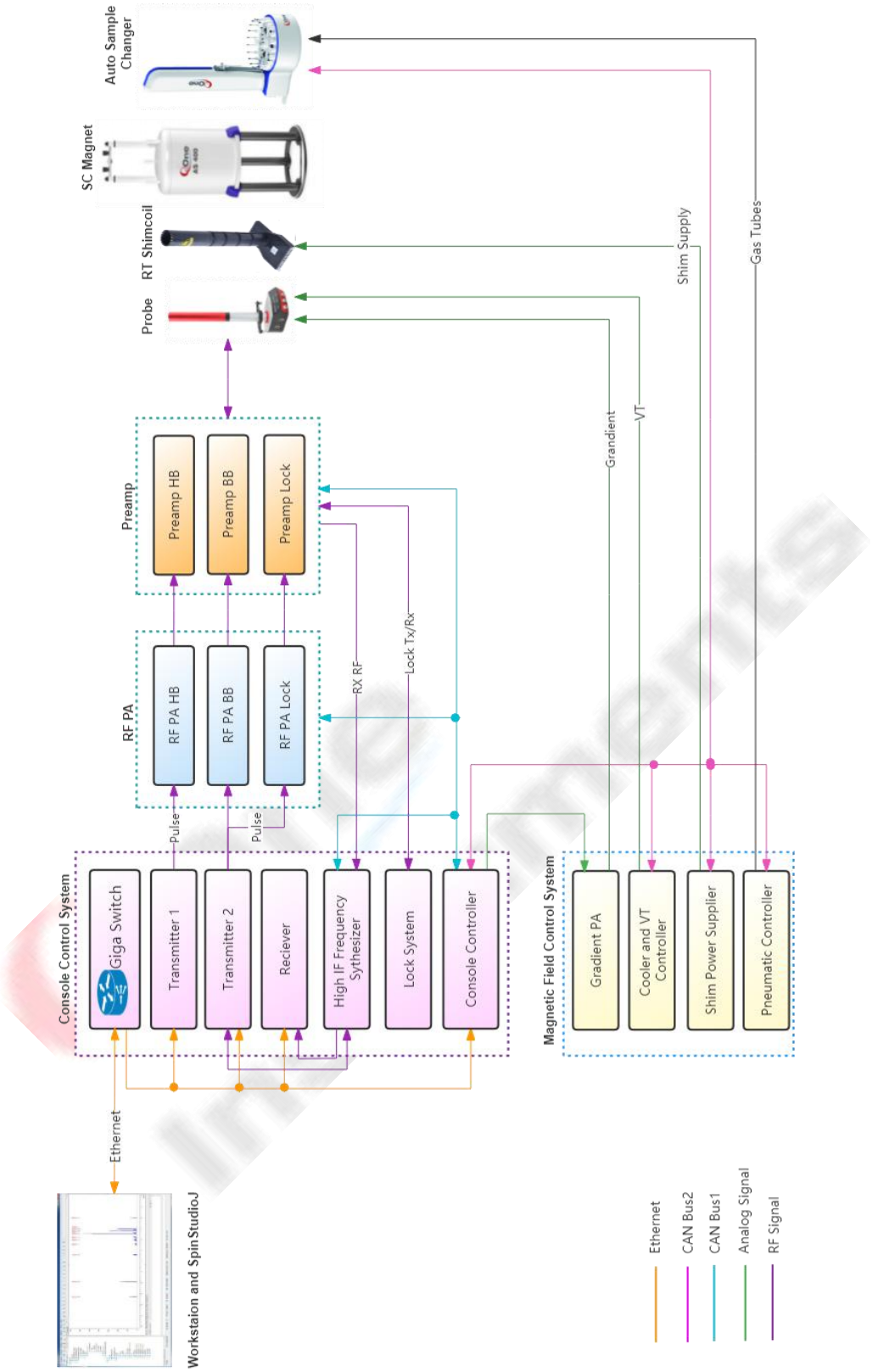


Fig. 2 Interconnection Diagram of Quantum-I Plus NMR Spectrometer

1.4.2 Superconducting magnet

The superconducting magnet consists of a dewar filled with liquid helium and liquid nitrogen and a superconducting coil. The vertical room temperature cavity in the center of the magnet is used to install the room temperature shim coil and probe. The basic structure of superconducting magnet is shown in Fig. 2.

Fig. 3 Superconducting magnet

Superconducting magnets provide a stable and uniform basic magnetic field for NMR spectrometers. Its specifications are usually expressed by the ^{1}H nucleus' resonance frequency corresponding to its magnetic field strength. For example, superconducting magnets with a

field strength of 11.7 T are expressed by the ^{1}H nucleus' resonance frequency of 500MHz. If the specification is followed by a size, the size generally represents the room temperature cavity diameter of the magnet, such as 500MHz/54mm.

Superconducting magnets are installed and energized at the user's site (commonly known as charging field). When the magnet system arrives at the site, each component is separated, and they are assembled at the site by Q.One installation engineer. After the magnet assembly is completed, the installation engineer will carry out all the work of magnet field energizing:

1) Vacuum pumping: The lower the vacuum degree of the magnet Dewar, the lower the volatilization rate of liquid nitrogen and liquid helium. It usually takes two to three days to vacuumize. In general, Q.One tries its best to vacuum the magnet to the lowest level to minimize the cost for users to refill liquid helium.
2) Pre-cooling: Fill the magnet with deep cold liquid nitrogen and liquid helium to make the superconducting coil enter a superconducting state. Pre-cooling is carried out immediately after vacuumizing is completed.
3) Energizing field and superconducting shim: within 5 hours after magnet precooling is completed, Q.One installation engineer will carry out energizing field and superconducting shim, which will take one to two days. When the field is in charging, there is a possibility the magnet may be quenched. Therefore, you should prepare enough liquid helium and liquid nitrogen to quench twice according to the requirements of the Installation Preparation Manual for Quantum-I*Plus* NMR Spectrometer. Once the magnet is quenched, the liquid nitrogen and liquid helium must be refilled as soon as possible, otherwise the magnet may be damaged.

After the magnet is installed, it takes 7-10 days to wait for the magnet to stabilize. During this period, the spectrometer is in an undelivered state, but the Q.One installation engineer may not be on site. You should assume the responsibility of the spectrometer supervision, check the Gaussian line range of the magnet, check whether the warning signs posted everywhere are complete, and prohibit all personnel and articles from approaching the

magnet according to the safety considerations in this manual, and prohibit moving or hitting the magnet.

After the magnet stabilizes, the Q.One installation engineer will test the spectrometer and finally deliver it to you for use.

1.4.3 RT shim coil

The room temperature shim coil is inserted from the lower direction of the room temperature cavity tube in the center of the magnet and fixed at the bottom of the magnet. The room temperature shim coil consists of 23-40 coils orthogonal to each other, and each coil is driven by one shim current channel of the magnetic field control system. Generally, the room temperature shim coil can improve the uniformity of the magnetic field to 1 ~ 2ppb to meet the requirements of high-resolution NMR experiments.

It should be noted that shim is not once and for all. The uniformity of the magnetic field will change with the external environment. Different samples will also have different effects on the magnetic field. In order to achieve the highest resolution, every time a sample is injected, it is necessary to re-shim again. In general, it is only necessary to fine-tune the first-order and second-order shimming on the basis of the original shimming value. It is not recommended for ordinary experimenters to adjust the high-order shimmer. Now you can also finish this work with the help of fully auto shimming function of SpinStudioJ.

The room temperature shimming coil has a cooling air pipe to pass airflow into the shimming coil to discharge the heat that may accumulate in the coil. Without the airflow, the shimming coil may be burned by overheating. The heat of shimming coil will be conducted to the sample at the same time, which will change the temperature of the sample and further affect the consistency of shimming and NMR experiment result.

1.4.4 Upper tube

Fig. 4 Upper tube

The upper tube is installed downward from the upper direction of the room temperature cavity tube of the magnet, and closely match with the top of probe in the center of the magnet.

The sample upper tube includes a set of pneumatic system to control the inject, eject and rotation of the sample and sensors to detect the rotation speed of the sample. When the sample is ejecting, the sample floats up to the top of the upper tube with the rotor under the pressure of the eject gas. During injecting, the flow rate of the inject gas slowly decreases, making the sample drop to the bottom of the u[per tube at a slow speed along with the rotor. When rotating the sample, there will be suspended air pressure at the bottom of the sample upper tube to support the rotor, so that the rotor is in a floating state, and under the action of horizontal rotating air pressure, the sample will rotate with the rotor at a certain speed. The control of suspended, rotating and injecting and ejecting gas is automatically controlled by the pneumatic controller.

The upper tube also includes a set of sensors for detecting the position of the sample, one

at the bottom of the upper tube and the other at the top of the upper tube. The top of the sample upper tube is provided with a circle of LED. When there is a rotor in the sample upper tube, the LED will be displayed in red, indicating that it is forbidden to put the sample again. When there is no sample in the upper tube, the LED will be displayed in green, indicating that the upper tube is free and a new rotter can be injected. The detection of the sample is real-time. Whenever the sample is put in, the color of the LED will be immediately converted to red.

CAUTION *Before the rotor is placed in the upper tube, the eject gas must be opened at first, untrained operators may cause sample breaking accidents by injecting the sample into the upper tube without opening the eject gas. Quantum-I Plus NMR spectrometer is intelligent to prevent the occurrence of such accidents. When a rotor at the top of the upper tube is detected, Quantum-I Plus NMR spectrometer will automatically open the eject gas to prevent the rotor from falling in.*

However, in any case, it is not recommended to put the sample into the upper tube without opening the eject gas. Developing this operation habit on Quantum-I Plus NMR spectrometer may lead to breaking the sample on other spectrometers.

1.4.5 Probe

Fig. 5 STM Probe

The probe is inserted from bottom to top from the central hole of the room temperature shim coil, the sample upper tube and the probe are closely matched in the center of the magnet, and the center of probe RF coil and the center of room temperature shim coil are aligned with the magnetic field center of the magnet. Installation and alignment of the upper tube and shimming coil shall be carried out by Q.One Installation Engineer.

It should be noted that during daily use, users should not try to adjust the position of the probe or rotate the direction of the probe. Inexperienced personnel may damage the probe or cause air leakage at the probe joint during this process, which will cause the sample tube to fall directly into the probe and the probe will be contaminated or even damaged.

If the spectrometer is equipped with several probes and needs to be replaced, only the probes need to be removed and the probes to be replaced need to be installed upward in the original direction. The position and direction of the fixed plane of the probe shall be corrected

by Q.One Engineer during installation. Please do not rotate or move the fixed plane of the probe up and down during use or storage. Please put the removed probe into the probe packing box for proper storage.

CAUTION *If the probe is contaminated, the probe must be removed. If you are not sure enough, please contact Q.One. If you disassemble the probe by yourself, we recommend that you use enough anhydrous alcohol (more than 500mL) to rinse the coil part of the probe repeatedly. Alcohol should not be used repeatedly. After rinsing, it should be placed vertically for more than 10 hours, the magnet should be reloaded, and the shim value should be adjusted before use.*

Each RF channel of the probe must be tuned to the acquisition frequency point before the experiment. The acquisition frequency of the manual probe can be adjusted by the tuning rods under the probe. Every RF channel has its own tune and match rods, and all rods are marked with labels of its corresponding RF channels. During tuning, only the rods of the tuning channel need to be adjusted, generally the tune rod should be adjusted at first, and then adjust the match rod, finally fine adjust both the the tuning and match rods as required. The automatic Smart Tuning and Matching(STM) probe can be tuned with the full-automatic tuning mode, also the tuning can be manually adjusted form the the SpinStudioJ software.

The glass dewar inside the probe is equipped with heater and thermocouples, which are connected to the VT controller in the console. The heater is located in the bottom of the glass dewar. When the heater is heated by current, the heat is brought to the position of the sample above the probe via VT airflow blowing into the glass dewar. The heating air flow is controlled by the pneumatic controller and displayed in SpinStudioJ. Please pay attention to observe whether it is normal.

There is a Flush gas port under the probe for inputting the cooling air flow for the probe coil and STM components. The air flow is automatically controlled by the pneumatic controller and displayed in SpinStudioJ. The airflow is directly blown to the RF coil to

prevent the temperature of the RF coil from changing and to ensure that the STM mechanism is kept in an appropriate temperature range.

The volume of VT and Flush airflow can be adjusted by SpinStudioJ. Please modify it as needed. It is generally recommended to set it to 10LPM. Too small airflow may lead to abnormal temperature control or probe function, and too large airflow may lead to sample disturbance.

1.4.6 Preamplifier System

Fig. 6 Preamplifier System

SPRA (Smart Preamplifier) is used to amplify NMR weak FID signals, so it is often placed very close to superconducting magnets. NMR spectrometer systems with different frequencies need to be equipped with different types of preamplifier systems.

The standard configuration of the preamplifier system includes 3 channels: high band channel, X channel and lock channel.

- High band channel: supports NMR experiments for nuclei with frequencies near ^{1}H and ^{19}F nuclei. In the standard configuration, this channel is connected to the HB interface of the probe through a high-pass filter.
- X channel: supports NMR experiments of all X nuclei in the $^{15}N \sim {}^{19}F$ nuclear range. In the standard configuration, this channel is connected to the X interface of the

probe through a low-pass filter.

- Lock channel: used for lock field and NMR observation of D core ~ ^{19}F core (lock field and observation cannot be shared, lock signal will disappear and lock field function will fail during observation). In the standard configuration, the lock channel is configured as D lock, which is connected to the Lock interface of the probe through the D band pass filter. When a ^{19}F lock is required, the filter needs to be replaced as a ^{19}F band pass filter.

If the spectrometer is equipped with more the 2 RF channels, the number of channels for X or high-band preamplifier can be increased.

All nucleus in the pass band of the high-pass filter of HB channel and the low-pass filter in X channel do not need to change the RF filters during observation and tuning.

1.4.7 Console

The Console Control Cabinet includes the core control components of Quantum-I Plus NMR spectrometer. After opening the front door of the cabinet, the components from top to bottom are as follows:

- CCS (Console Control System): includes receiver (RECV.xx), transmitter (TRSM.xx), main control board (MSTR.xx), lock board (LK.xx), clock board (CLK.xx), frequency source, router and power supply installed at the back of the chassis.

  1Gbps high-speed router provides high-speed communication connection between receiver, transmitter, main control board and the NMR workstation. The frequency synthesizer includes a two-channel transceiver integrated frequency synthesizer for generating transmitted pulse signals and received intermediate frequency signals.

- RF power amplifier: used to amplify the pulse signal output by the transmitter, which has high linearity and high harmonic suppression ratio and meets the requirements of

complex nuclear magnetic resonance pulse sequences.

Note that the maximum power of different RF power amplifiers is significantly different. It is forbidden to use high-power power amplifiers on low-power spectrometers, which will lead to the danger of burning the probe.

- Magnetic Field Control System (MFCS): includes a gradient power amplifier, a room temperature shim system with up to 40 channels (composed of TR # Rx.xx, AX.xx and Z0.xx), an pneumatic control system, a VT controller and power suppliers for all the boards.

Fig. 7 Internal Components of Quantum-I Plus Cabinet

The shim system is controlled by the rightmost shim control board (CTL.xx), which receives the shim setting parameters from CAN bus and controls each channel board to output the specified current.

The pneumatic control board is installed at the rear of the chassis to complete sample ejection, injection, rotation, bearing, VT control airflow and probe flush airflow control of the probe, and has the functions of monitoring the air pressure and humidity of the input air source to prevent spectrometer failure caused by insufficient input air pressure or excessive humidity.

The VT controller is built with the liquid nitrogen cooler driver, which is used to drive the liquid nitrogen volatilization refrigerator to complete the refrigeration function. When the spectrometer is equipped with the liquid nitrogen refrigerator, the cryogenic controller is installed at the rear of the chassis.

The power supply system is installed at the rear of the chassis and consists of a transformer, several power supply boards for all boards.

1.4.8 NMR workstation

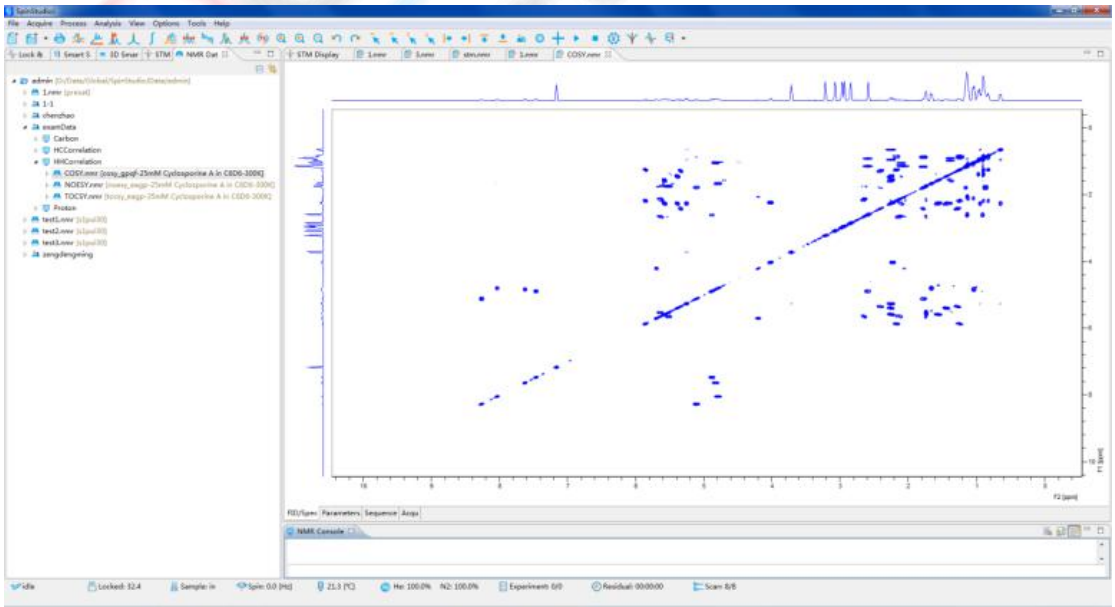


Fig. 8 SpinSdudioJ Control and Data Processing Software

The NMR workstation includes a workstation with Windows or Linux operating system installed, and the NMR spectrometer control and data processing software SpinSdudioJ installed in the workstation.

The users of Q.One NMR spectrometer control the spectrometer system to carry out NMR experiments or process experimental results through SpinSdudioJ software. The contents displayed by the software include graphical pulse sequence, FID, spectrum, spectrometer working status, etc.

1.5 Product Dimensions and Installation Space Requirements

1.5.1 Size of control cabinet

The standard configuration of Quantum-I Plus NMR spectrometer is dual-channel single-door cabinet. Multi-channel cabinet is another customizable cabinet. Users can choose dual-door cabinet or higher single-door cabinet according to customized requirements.

The size of the cabinet is (mm): 650 × 980 × 1200.

Total weight (kg): 204.4.

Material of control cabinet: stainless steel.

Surface treatment: Insulation plastic spraying.

1.5.2 Size of superconducting magnets

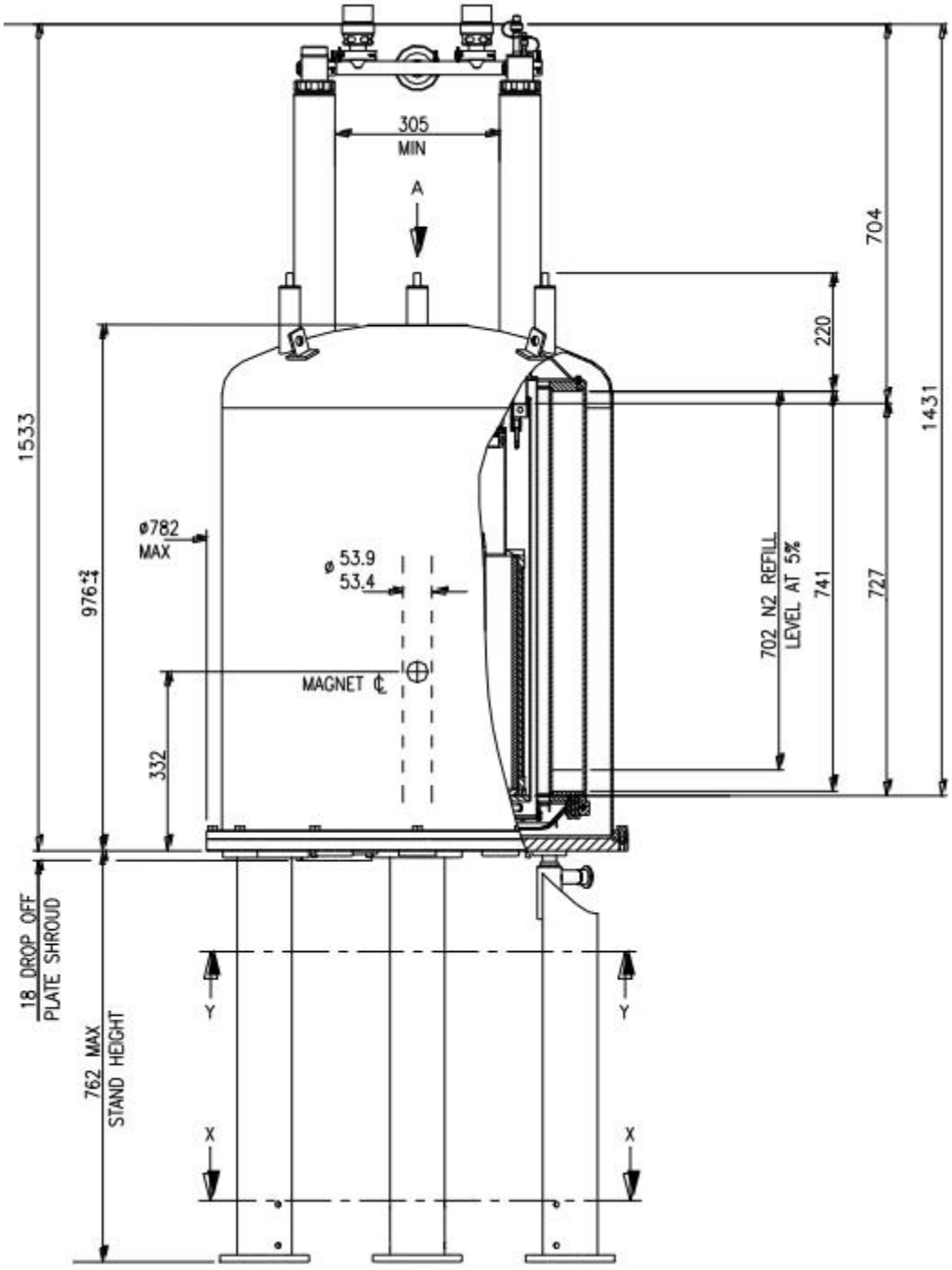


Fig. 9 AS400 Superconducting Magnet Dimensions

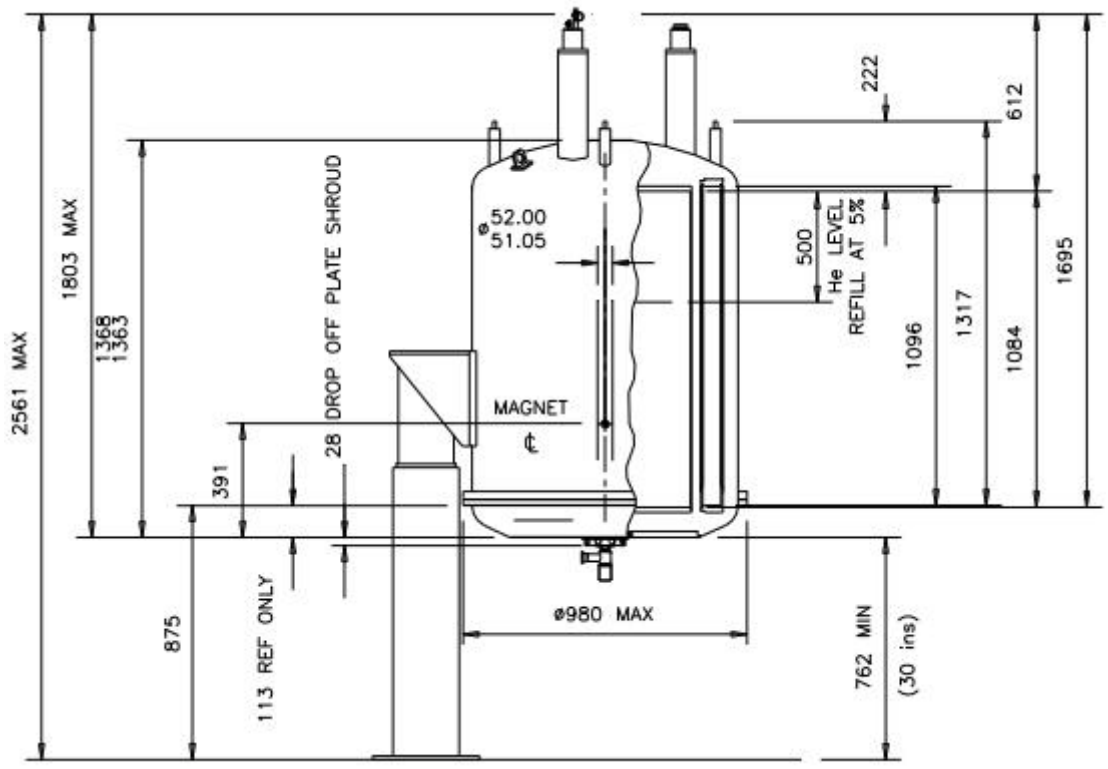


Fig. 10 AS600 Superconducting Magnet Dimensions

1.5.3 Dimensions of other components

Some components of Quantum-I Plus NMR spectrometer cannot be accurately written down in this product manual, because they are mostly components configured by users themselves or purchased from third parties, such as worktables, cabinets, chairs, air compressors, air conditioners, etc.

When considering the installation position, users should ask the third party for the dimensions of the components provided by them. Air conditioners, chairs, worktables, etc. can be arranged according to the standard dimensions.

1.5.4 Requirements for installation space

Nuclear Magnetic Resonance Spectrometer is a huge and complicated system. The main components to be installed include console, superconducting magnet, worktable, air compressor, cold dryer, UPS, air conditioner, etc. Superconducting magnet has a certain stray field range, and a certain space must be reserved around it.

Generally, it is necessary to use two rooms to install the nuclear magnetic resonance spectrometer, one room is used to install the air compressor and its attached cold dryer, air storage tank, etc., and the other room is used to install the console, worktable, superconducting magnet and their attached components.

When installing the nuclear magnetic resonance spectrometer, the requirements of floor load bearing, non-magnetic environment, electromagnetic wave interference limit, power supply stability, temperature stability control, etc., as well as the influence of the equipment on other objects, people or equipment, room location, space layout, etc. need to be strictly considered and designed.

Q.One provides "Quantum NMR Spectrometer Installation Preparation Manual" and "Quantum NMR Spectrometer Installation Condition Confirmation Form". The document lists the installation requirements of nuclear magnetic resonance spectrometer in detail. Please prepare the installation conditions according to their requirements.

1.6 System Compatibility

Quantum-I Plus NMR Spectrometer is not necessarily compatible with different superconducting magnets. Q.One does not provide guarantee for customers to change or modify the use of Quantum-I Plus NMR Spectrometer. Such behavior of users will cause Q.One to terminate the guarantee service provided to users. The following is a description of the compatibility of the Quantum-I Plus NMR spectrometer and is not a hint or warranty of Q.One as to the potential use of the system.

Most of the components of the Quantum-I Plus NMR spectrometer are fully compatible with the control software, and can be directly used for system control equipped with 200MHz-600MHz superconducting magnets. These compatible components include: the main console (CCS) all other components except the field frequency interlocking system (LK.xx) and the magnetic field control system (MFCS). The control software SpinStudio can be used for any model of Quantum-I Plus NMR spectrometer, but its configuration file needs to be changed.

The following components are incompatible in different types of systems: the field

frequency interlocking system (LK.xx) of the main console (CCS), the forward amplifier system (PAS), the probe and the superconducting magnet.

Other components, such as RF power amplifiers, have certain backwards compatibility according to their specific models. Q.One provides upgrade and modification services based on the existing system. According to your needs, Q.One will replace or upgrade some components to achieve the expected functions. Please consult Q.One for details.

1.7 System Performance Indicators

1.7.1 Indicators of control system

Please refer to the public index description document officially issued by Q.One for details of the performance index of the control system of Quantum-I Plus NMR spectrometer.

1.7.2 Probe performance index

The performance index of the probe varies according to the probe model. For details, please refer to the public probe performance index description document officially issued by Q.One.

1.8 System Security Risks

1.8.1 Security Risk Identification

Strong magnetic field will cause potential safety hazards to specific objects and personnel. Anyone who may approach NMR spectrometer should understand these hazards and take careful precautions during system installation and use. The following figure lists the range of diffusion fields for various magnets. It should be noted that the data listed in these charts are standard values, and the actual diffusion field range of each magnet may be different, so each magnet should be tested after installation.

Cardiac pacemaker carriers must be prevented from entering areas of strong magnetic fields that may generate danger. For example, in the floor, a certain space is reserved for the area directly above and directly below the magnetic field. When determining the harm of the system to the cardiac pacemaker, please consult the user manual of the cardiac pacemaker, contact the manufacturer of the cardiac pacemaker, or consult a doctor for help.

Q.One has equipped each system with a warning sign for the danger of strong magnetic field. For detailed explanation and posting requirements of various signs, please refer to the "Posting Requirements for Safety Signs with Strong Magnetic Field" section for details.

Since the magnetic field of the magnet exists in both horizontal and vertical directions, the influence of the magnetic field on personnel, electronic equipment, computers, etc. above and below the magnet must be considered. Strong magnetic field warning signs may also need to be posted on adjacent upper or lower layers. The following figure shows the standard magnetic field values of 400MHz and 600MHz magnets in the vertical direction.

If you have additional posting label requirements, please contact Q.One.

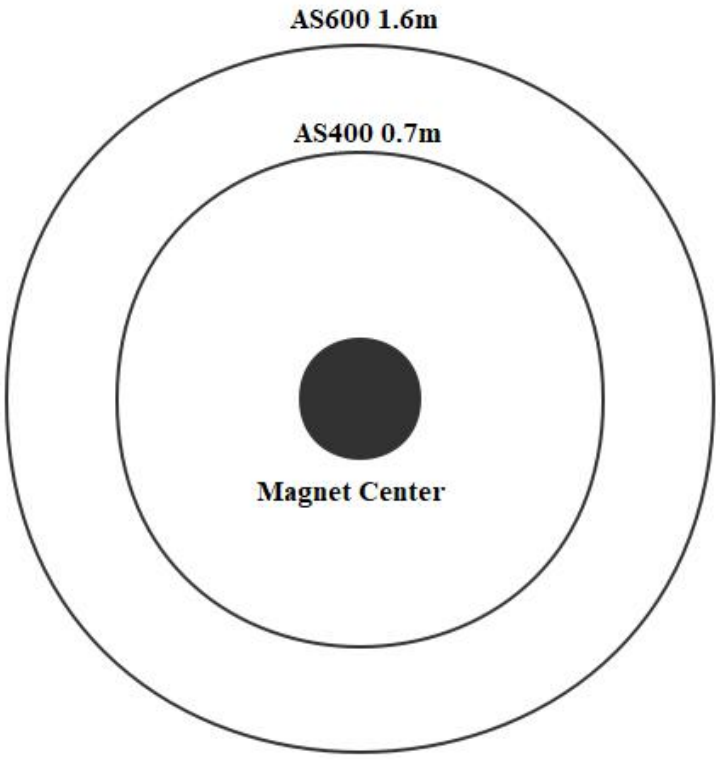


Fig. 11 Typical 5 Gauss Magnetic Field Range (m) of Magnet

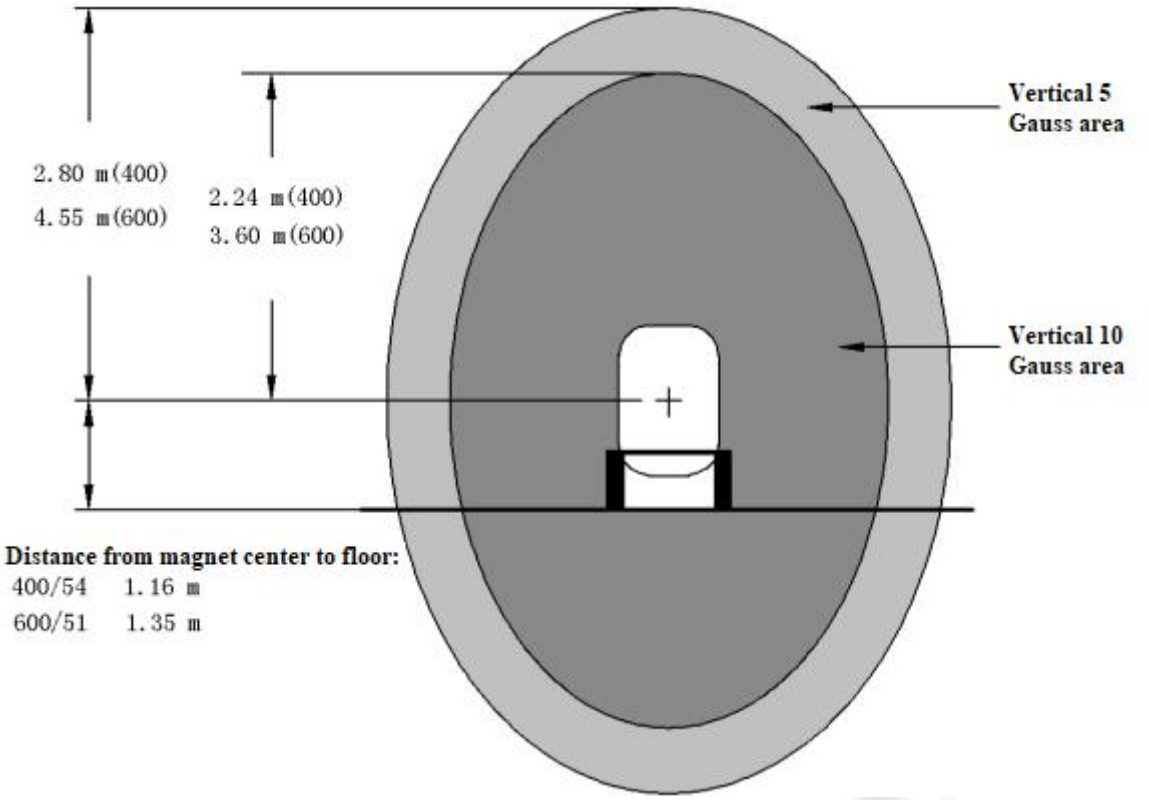


Fig. 12 Vertical magnetic field distribution of different magnets

1.8.2 Safety of personnel

NMR experimenters are directly exposed to high-intensity static magnetic fields, but so far, there is no conclusive evidence to prove that magnetic fields that do not exceed the magnetic field strength of NMR spectrometers will cause harm to human bodies. The common magnetic field strength of NMR spectrometer is shown in Table 4.

Table 2 Diffusion field ranges for different magnets

Magnet type (MHz/mm)	Horizontal Distance (CM)			Vertical Distance (CM)			Ground to Centerline Distance (CM)	Distance from magnetic field edge to centerline (CM)
	0.6 kG	6 kG	20 kG	0.6 kG	6 kG	20 kG		
AS600	70	*A*	*A*	96	48	35	44.0	45.9
AS400/54	39	*A*	*A*	59	*B*	*B*	33.2	36.2

Note: a. The horizontal distance point is located inside the magnet.

b. The vertical distance point is located inside the magnet.

Some studies suggest establishing the relationship between magnetic field and reproductive health, but the medical data obtained so far are not sufficient to prove that magnetic field has definite influence on reproduction or pregnancy. In other words, the current scientific conclusion does not support the view that the static strong magnetic field of NMR spectrometer is dangerous to reproduction or pregnancy. It can be considered that the static magnetic field of NMR spectrometer is harmless to human body. The article "Threshold Limit Values and Biological Exposure Indices, 5th ed." Published by the National Industrial Health Association of the United States has the following statement:

- TLVs (Safety Limit Value) refers to the flux density of static magnetic field that does not cause health hazards to workers frequently exposed to static magnetic field. This value is used to guide the control of exposure to static magnetic field, but cannot be used as a criterion to measure danger and safety.
- When exposed to a static magnetic field for a long time, the whole body shall not exceed 60mT (600 Gauss), or the average working day (8 hours) shall not exceed 600mT (6000 Gauss). The maximum flux density of the magnetic field is 2T (20,000 Gauss).

1.8.3 Other safety instructions

Although the strong magnetic field of superconducting magnet is the most dangerous part of NMR spectrometer, there are still other parts of the whole system that may have possible safety hazards, which may lead to damage to spectrometer or personnel. In particular, laboratory administrators or operators should have full understanding of this.

1) High voltage

Quantum-I Plus NMR spectrometer uses 110V or 220V AC power supply, and high voltage is distributed throughout the rear of the cabinet and inside each cabinet, as well as UPS and wiring outside the cabinet.

All power sockets of Quantum-I Plus NMR spectrometer are pluggable. During daily use or maintenance (such as cleaning the interior of the cabinet), the power socket may be

unplugged or loosened accidentally, and the conductor with 220V power supply may also be exposed, causing potential potential safety hazards of power cord ignition or electric shock.

If the ground wire connection in the laboratory is not normal, it may also electrify the cabinet, make the equipment unable to work normally, reduce its performance, and may bring potential personal safety hazards.

Laboratory administrators should often check whether the contact of each power cord is firm and whether the insulation seal is in good condition to ensure that the strong power part will not be intentionally or unintentionally contacted and the grounding wire is connected reliably.

2) Radio frequency field

Quantum-I Plus NMR spectrometer has a large number of RF emission sources, which are safe because of wired connection and reliable cabinet shielding. However, in the case of RF cable falling off, damage or incomplete cabinet, RF radiation hazards may be caused. During use or maintenance, no one should attempt to remove or switch any cables of the system, nor should he take any act that damages the integrity of the cabinet, such as removing the cabinet door. Laboratory administrators or spectrometer users should pay attention to check whether the cables are connected reliably to avoid problems such as loosening and falling off of the cables, and the cabinet should also be intact.

When the cabinet door and the cabinet are closed, the cabinet can form a shield of radio frequency field to prevent the radio frequency field inside the cabinet from radiating outward and prevent the external radio frequency field from entering the cabinet. When the cabinet door is opened, the RF protection function of the cabinet will be completely lost. At the same time, in order to ensure the safety of operators, the fan will stop running when the rear door of the cabinet equipped with the fan is opened. When there is no fan to dissipate heat from the cabinet door, the heat inside the cabinet will gradually accumulate and the overall performance will gradually decline. Therefore, under any circumstances, the cabinet door should be kept closed, which not only ensures the radio frequency shielding performance, but also ensures the normal operation of the internal heat dissipation system of the cabinet.

3) Cryogenic liquid

Cryogenic liquids such as liquid nitrogen and liquid helium exist in large quantities in superconducting magnets of NMR spectrometers, which are safe under normal conditions, but dangerous under specific conditions.

Note that when cryogenic liquid contacts human body, the effect is the same as that when human body contacts extremely hot objects. When liquid nitrogen is filled, the liquid nitrogen will overflow after being filled, causing severe burns when contacting the skin, and causing serious consequences such as blindness when contacting weak parts such as eyes. The temperature of the transmission tube for transporting cryogenic liquid is very low, and the human body will stick to the skin when contacting it. Attempts to remove it will tear the skin. The temperature of liquid helium is lower, it will vaporize violently when it comes into contact with air, and the temperature near the outlet of liquid helium is also very low. Therefore, the filling of cryogenic liquid needs to be carried out by personnel with rich experience in cryogenic liquid treatment, and unqualified laboratory managers or spectrometer operators are prohibited from contacting cryogenic liquid.

When filling cryogenic liquid, special attention should be paid to the fact that the cryogenic liquid does not splash on any part of the magnet, which will cause the magnet to lose excess.

4) Hypoxia

Hypoxia is a potential danger in NMR laboratories, especially in laboratories with narrow space. Liquid nitrogen and liquid helium in superconducting magnets are constantly volatilizing, which will reduce oxygen in the room. When filling liquid nitrogen and liquid helium, a large amount of volatile liquid will significantly reduce indoor oxygen. At this time, doors and windows should be opened, or air conditioning and other equipment should be used to supply air to the room to keep the room free from oxygen deficiency.

The worst case is that when the magnet loses time, the magnet will lose time under the conditions of impact, insufficient liquid helium, vacuum leakage, etc. At this time, a large amount of gas (liquid nitrogen and liquid helium) will be rapidly ejected from the magnet, and

the oxygen in the room will disappear rapidly. At this time, all personnel in the room should withdraw immediately and cannot return until the oxygen in the room returns to the normal level. It is recommended to install an oxygen monitor in the nuclear magnetic resonance laboratory.

5) Fire

Aging cables, loose joints and rat infestation may cause cable fires. Smoking in the laboratory, splashing conductor liquids such as fire, mineral water and beverages into sockets, cabinets and workstations may cause short-circuit fires and serious consequences. Therefore, laboratory administrators should strictly manage, prohibit beverages, food, pets, etc. from being brought into the laboratory, and regularly check whether cable protection is safe.

The laboratory administrator should organize necessary fire drills. Don't panic in case of fire. Use non-magnetic fire extinguishers to put out the fire. If you are at a loss, you should evacuate the laboratory immediately.

6) Uncontrollable factors

Uncontrollable factors include earthquakes, terrorist attacks, wars, etc. Under the condition of ensuring personal safety, we should try our best to protect the laboratory, properly keep toxic and volatile articles, reliably isolate strong magnetic field areas, and prevent unauthorized personnel from accidentally approaching magnets.

2 Installation

2.1 Installation Preparation

2.1.1 Installation environment preparation

The preparation of the installation environment refers to the process in which you should select and prepare the environment and facilities for the installation of the spectrometer system before it arrives at the installation site.

The preparation content generally includes:

(1) Site selection: i.e. Select an installation space with minimum interference to the magnet. The selection of an optimal site depends on the edge area of the high magnetic field of the system. Due to the interaction between the magnetic field of the system and the surrounding environment, the selection process may be very complicated.

Please refer to Q.One's "Quantum NMR Spectrometer Installation Preparation Manual" for details to be considered when selecting the installation site. Before installing the Quantum-I *Plus* NMR Spectrometer, Q.One will send an installation engineer to confirm with you whether the installation site meets the requirements. Please carefully check the installation site and conditions according to the requirements set forth in the document, truthfully fill in the "Quantum NMR Spectrometer Installation Condition Confirmation Form" and feed back to Q.One. Please keep in close contact with Q.One when preparing the installation site. If you have any questions, please consult Q.One.

(2) Power supply: refers to the power supply that the laboratory shall provide to Quantum-I Plus NMR spectrometer, air compressor, dryer, air conditioner, dehumidifier and other equipment. The power supply to be provided includes several 110V ~ 220V single-phase power supply and 380V/50Hz three-phase power supply. At the same time, special grounding wires shall be provided for Quantum-I Plus NMR spectrometer.

Some parts need you to provide, such as tables and chairs, hot blower, heat insulation gloves, etc., which need you to purchase in advance.

Attention should be paid to ensuring that the nuclear magnetic resonance laboratory has

sufficient power supply and cannot be cut off frequently. Frequent power cut-off will cause the failure of magnet field lifting, bringing unnecessary economic losses or additional expenses. Unexpected power cut-off may also cause damage to Quantum-I Plus NMR spectrometer.

In general, accidental power failure is inevitable. UPS is essential to NMR spectrometer. NMR spectrometer should match UPS with sufficient power and battery capacity. When using UPS, it should be noted that if the power failure is too long, it may exceed the battery power supply time of UPS. At this time, the spectrometer should be manually turned off in advance.

（3）Gas source: The gas source is used to drive the suspension, entry, exit and rotation of the sample, as well as the suspension of the magnet, the cooling of the room temperature shimmer coil, the heating of the sample, etc. The air pressure of the gas source shall be greater than 90psi (0.62 MPa), the air flow rate shall not be less than 100L/min, and the gas shall be fully dried without any oil content. Therefore, in general, you should install a cold dryer for your oil-free air compressor. Attention should be paid to the large amount of water in the storage tank of the air compressor. The air compressor should drain water every day to make room for air and prevent the water in the air source from exceeding the standard. It is suggested to install timing automatic drainage device for air compressor.

In order to ensure stable air flow, especially when multiple systems use one air source at the same time, you should install a gas storage tank with a large enough volume for the system.

The compressed air shall be re-filtered and used before entering the Quantum-I Plus NMR spectrometer. Q.One provides a set of filtering devices. It should be ensured that the filtering devices are connected normally and whether the filters are effective or not should be observed. The filters should be replaced regularly.

The Quantum-I Plus NMR spectrometer is equipped with a humidity monitor. When the humidity of the input gas exceeds the limit, the pneumatic system will stop working and report the humidity exceeding the limit through SpinSdudioJ.

(4) Forklift: When the system equipment arrives at the installation site, you need a

forklift to unload and transport it to the installation site. The forklift truck shall have a load of more than 1 ton and can rise to a height of 1.5 meters and a width of less than 0.77 meters.

Special attention should be paid to the selection of the installation site. There should be no steep slopes, thresholds, steps, etc. in the transfer route from the unloading site to the installation site so that forklifts can pass without obstacles.

(5) Non-magnetic steps, worktables, seats, lockers, wiring rows and other supporting components are provided by you. These components are described in detail in the "Quantum-I Plus NMR Spectrometer Installation Condition Confirmation Form". Please fill in the form together and feed back to Q.One.

The Installation Preparation Manual for Quantum-I Plus NMR Spectrometer provided by Q.One describes the installation conditions of Quantum-I Plus NMR Spectrometer in detail, while the accompanying Confirmation Letter for Installation Conditions of Quantum-I Plus NMR Spectrometer lists the inspection contents of installation conditions item by item. Please carefully check the installation site and conditions, truthfully fill in the Confirmation Form for Installation Conditions of Quantum-I Plus NMR Spectrometer and sign for confirmation.

If you have signed the "Confirmation Form of Installation Preparation Conditions for Quantum-I Plus NMR Spectrometer", Q.One believes that the installation site has met all the conditions required for the installation of the spectrometer system as specified in the "Specification Form for Installation Preparation Conditions for Quantum-I Plus NMR Spectrometer". Q.One will not be responsible for the delivery delay or additional economic losses caused by insufficient installation conditions.

2.1.2 Preparation of installation materials

Q.One Installation Engineer needs the following supplies during the installation process, and you should prepare them completely before installation:

- Liquid helium supply: > 300L.

- Liquid nitrogen supply: > 300L.
- High pressure helium, purity > 99.99%, pressure > 16MPa.
- High pressure nitrogen, purity > 99.99%, pressure > 16MPa.
- Alcohol.

The supply of liquid helium and liquid nitrogen is particularly important. Please make arrangements as soon as possible after ordering the spectrometer and ensure continuous supply during the initial delivery and operation.

Alcohol is not less than 500mL and is used to clean spectrometer components. Be careful not to use acetone, which will damage the plastic and paint of the spectrometer.

2.2 Signing for packing boxes

The number of NMR spectrometer packing boxes sent by Q.One will vary according to the number of components. In order to facilitate your acceptance, each packing box is numbered sequentially in the form of "serial number/total number" and is accompanied by an internal goods list.

The packing box number and cargo list shall be consistent with the contents of the "Quantium-I Plus NMR Spectrometer Packing List" sent to you by Q.One. Please carefully check the received goods according to the "Quantium-I Plus NMR Spectrometer Packing List" and type "√/×" one by one for confirmation. If there is any problem in the inspection, please type "" in the corresponding confirmation column and take photos to record it. Please sign the name and date after signing, and feedback the signing result to Q.One in time. When Q.One installation engineer arrives, please forward the completed "Quantum-I Plus NMR Spectrometer Packing List" to them.

All packing boxes are posted with obvious signs. Except for signs that are afraid of dampness and fragility, packing boxes with strict requirements on inclination and vibration are all marked with anti-inclination and anti-vibration signs. When receiving and inspecting goods, special attention should be paid to whether these signs are abnormal.

When signing for the receipt, please pay attention to check the following:

- The appearance of the packing box shall be intact and free from traces of impact, pressure and moisture.
- The Shock Watch label of the packing box shall be colorless.
- The tilt angle of the TILT Watch label on the packing box shall be less than 30 °.

WARNING *If the appearance or label of the packing box is abnormal, please take photos and contact Q.One.*

WARNING *Personnel who are not authorized by Q.One shall not open the package without authorization, and the losses caused by unauthorized acts shall be borne by the customer.*

2.3 Unloading, Transshipment and Storage

Quantum NMR spectrometer packing boxes are different in size and weight. Wooden bases are installed at the bottom of heavier packing boxes to facilitate forklift transportation, while lighter packing boxes can be directly transported by manpower.

During unloading and transfer, please be sure to pay attention to the reminder signs of the packing box, such as inclination angle, vibration, etc., and pay attention to the following matters:

- All packing boxes shall be transported and stored upright.
- Handle with care and do not hit or fall any packing box.
- No articles exceeding the limit of stacking layers shall be stacked on the packing box. In principle, only one layer of lighter paper packaging articles is allowed to be superimposed on the paper packaging box, two layers of lighter aluminum alloy packaging articles can be superimposed on the aluminum alloy box, and one layer of paper or aluminum alloy box packaging articles can be superimposed on the wooden packaging box.
- Packing with inclination angle restriction shall be transported and stored strictly

vertically.

- Packages with vibration limitation shall be lifted and handled lightly and shall not collide with other articles.

After unloading, after you sign for it, you should store all items in a room with strict temperature and humidity control. The temperature and humidity should meet the following conditions:

- Temperature: 16 ~ 27 ℃.
- Humidity: 40% ~ 60%.

At the same time, the room should be dustproof, waterproof and fire-proof measures.

Please notify Q.One to schedule the installation time after the storage of the items is completed.

2.4 System Installation

This section describes the steps and contents of the installation of Quantum-I Plus NMR spectrometer according to the workflow. All the installation processes are mainly completed by Q.One installation engineers. You are not normally required to participate except for possible consultation or assistance.

2.4.1 Magnet installation

The installation of the magnet includes:

- Determining the installation site of the magnet.
- Fixing the pneumatic strut.
- Install the magnet.
- Install room temperature shim coil and probe.

When determining the installation site of the magnet, it is necessary to determine the installation position of the control cabinet, worktable at the same time, i.e. To determine the

arrangement of the laboratory. Q.One generally gives priority to the arrangement scheme you provided when preparing the installation conditions. Once confirmed, the magnet will be fixed and forbidden to move. The control cabinet and workbench should be placed outside the specified 5 Gauss line range. The front placement system should be placed as close to the magnet as possible. You can adjust it yourself.

2.4.2 Vacuum pumping

Vacuum pumping finally makes the vacuum of the magnet reach more than 2×10^{-5} mbar, which is expected to take three to four days.

2.4.3 Pre-cooling with liquid nitrogen and liquid helium

The pre-cooling of the magnet includes the following steps:

(1) Fill liquid nitrogen into the liquid nitrogen vessel after the magnet vacuum reaches the target.

(2) Pre-cooling the liquid helium vessel with liquid nitrogen.

(3) Using dry high purity nitrogen and high purity helium gas to replace precooled liquid nitrogen in the liquid helium vessel.

(4) After the replacement is completed, liquid helium is filled into the helium vessel.

(5) Filling the liquid helium vessel with liquid helium and filling liquid nitrogen to the nitrogen vessel.

(6) Wait for a few hours to allow the magnet to cool sufficiently before proceeding to the next step.

Pre-cooling and filling of liquid nitrogen and liquid helium is a step-by-step process that takes about 2 days.

2.4.4 Energizing and superconducting shim

Before energizing the magnet, a vacuum cleaner or magnet should be used to clean the laboratory floor to prevent ferromagnetic impurities from being adsorbed into the magnet after energizing.

The installation engineer uses the power supply to charge the field of the magnet, and uses the superconducting shim power supply to carry out superconducting shim, so that the field strength of the magnetic field reaches the specified strength and sufficient uniformity. The better the uniformity of the basic field, the easier it will be for users to carry out room temperature shimming during use. Therefore, Q.One installation engineers will ensure that the work is carried out carefully and carefully and adopt various methods to improve the uniformity of superconducting magnetic field as much as possible.

The process of energizing the magnet and superconducting shim takes about 3 days.

2.4.5 NMR workstation installation

Q. One's workstation delivered with the whole spectrometer has been installed and can work after the cables are connected at the work site.

If the workstation is provided by you, the contents that need to be installed in the workstation include:

(1) Connect a computer.

(2) Install the operating system.

(3) Install SpinSdudioJ.

(4) Install auxiliary software.

SpinSdudioJ requires parameter configuration after installation. Please note that the configuration files are backed up for quick recovery when software is upgraded or workstations are replaced.

2.4.6 System Connection

The connection of system cables includes the connection of workstations, superconducting magnets, upper tube, cables and other parts between the preamplifier system and the control cabinet.

2.4.6.1 Gas tube connection

See the following figure for gas tube connection diagram. Connections include:

(1) Connect the gas pressure regulating valve and the Gas In interface of the pneumatic control system with a 10mmgas tube.

(2) Three 6 gas tubes are used to connect the Bearing, Rotation and Eject interfaces of the pneumatic control system and the Bearing, Rotation and Eject interfaces of the upper tube.

(3) Connecting the VT Gas and Flush Gas interface of the pneumatic control system to the VT gas and Flush gas interface of the probe with two 8mm-6mm gas tube adapters.

(4) Use 2 6mm gas tubes to connect the pressure regulating valve and room temperature shim coil cooling, magnet air floating leg and automatic sample changer. Pay attention to connecting throttle needle valves in series in the middle of the gas tube connected with the room temperature shimming coil, and carefully adjust the air flow according to the total power and heating volume of the room temperature shimming coil to maintain the temperature of the room temperature shimming coil at the normal level.

(5) In order to avoid misoperation in daily use, the input port of the gas filter is equipped with a general pressure regulating valve. Please adjust it to an appropriate range to limit the maximum atmospheric pressure of the rear gas components.

(6) The air pressure of each passage of gas output by the filter needs to be carefully adjusted. This work is completed by the installation engineer during installation. Please pay attention to recording the value of each passage of air pressure so as to facilitate readjusting the air pressure during subsequent maintenance.

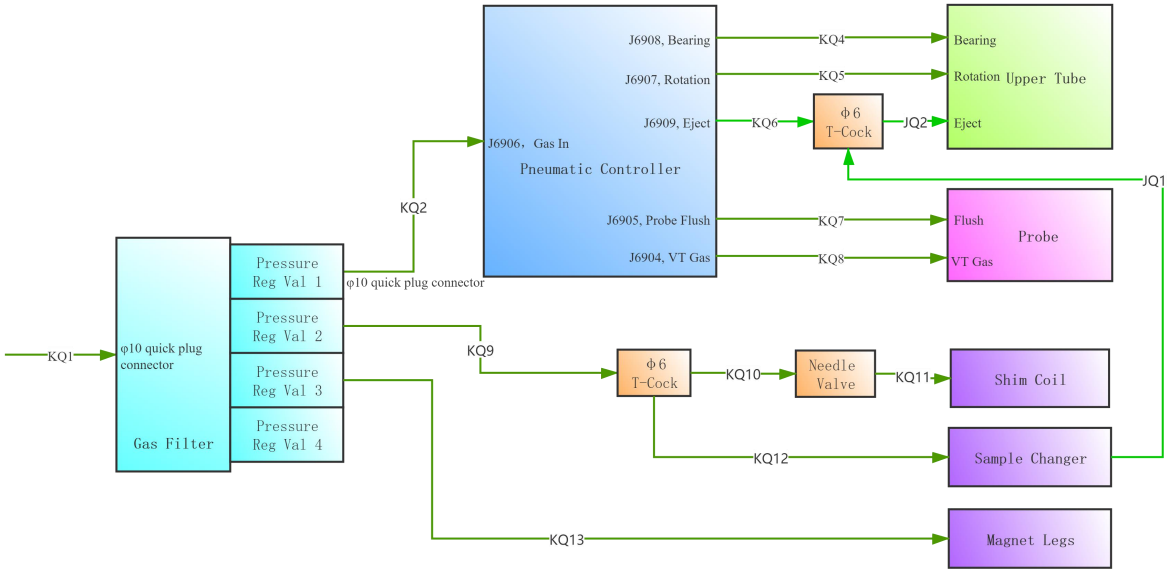
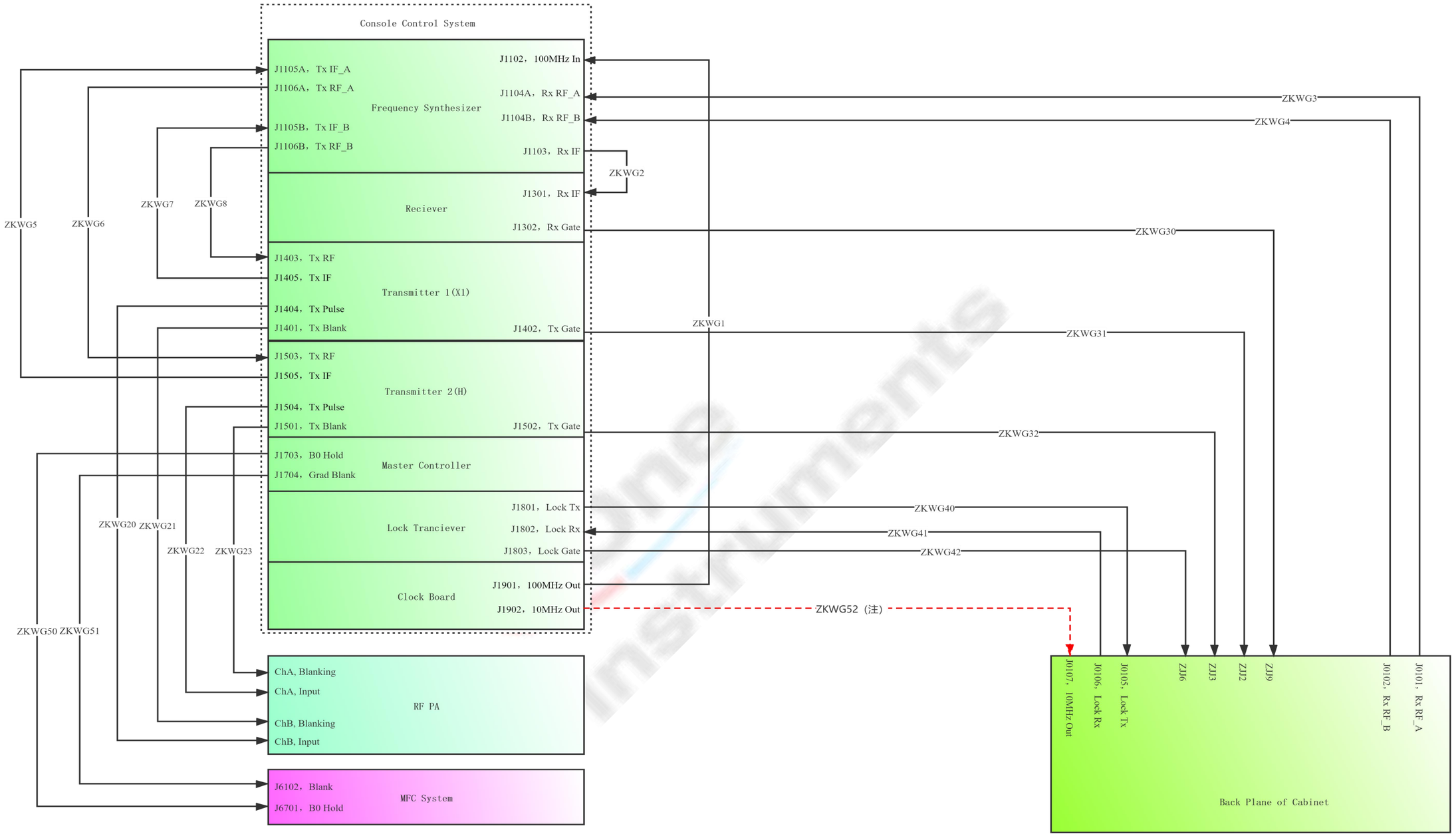


Fig. 13 Diagram of gas tube connection

2.4.6.2 Cable connection

All cables of Quantum-I Plus NMR spectrometer have obvious interface marks at both ends. Just insert the cables into the corresponding interfaces according to the following figure.



Note: Cable ZKWG52 is optional, install this calbe when the VNA is installed in the Preamplifier.

Fig. 14 2 Channel Cabinet Internal RF Cable Connection Diagram

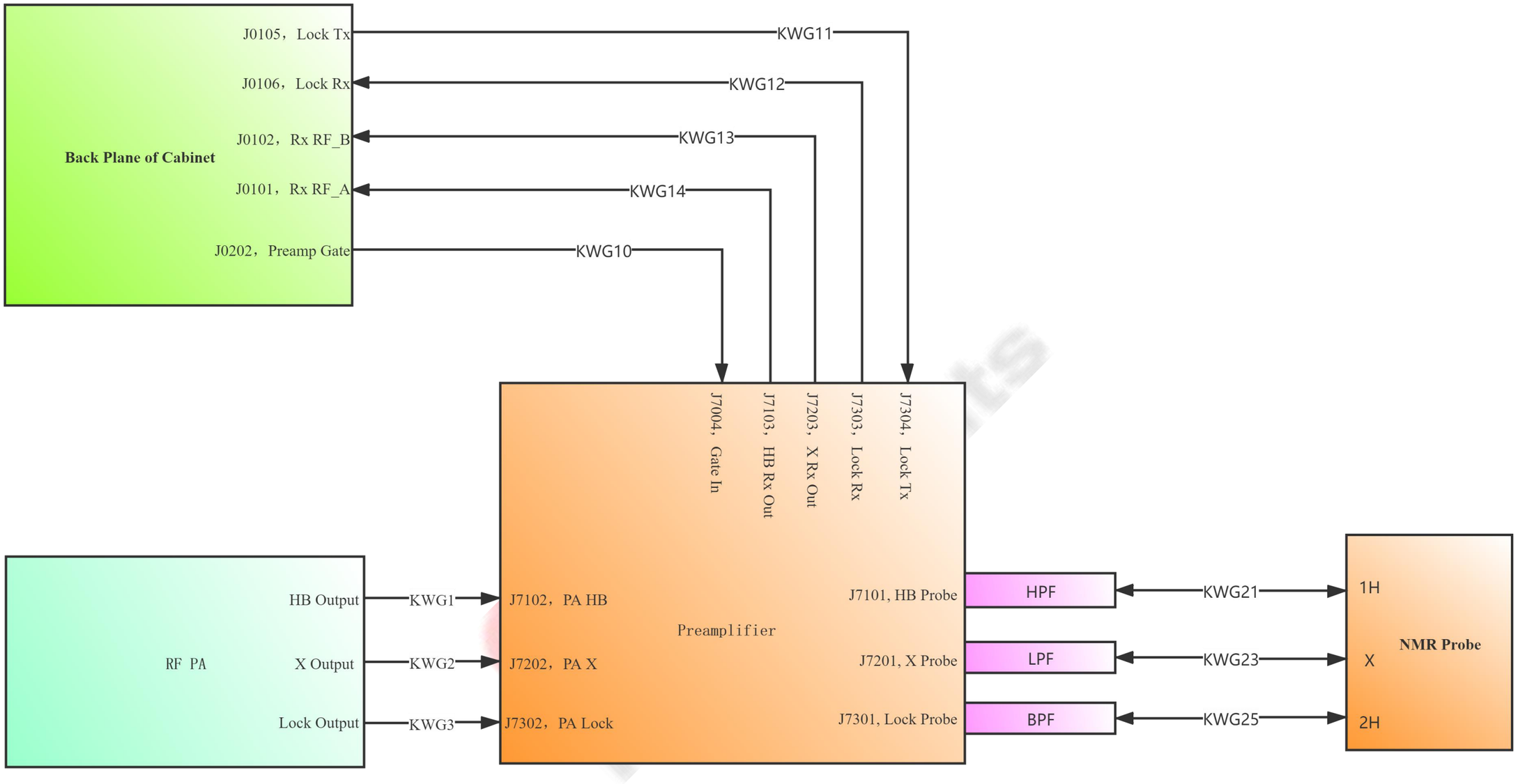
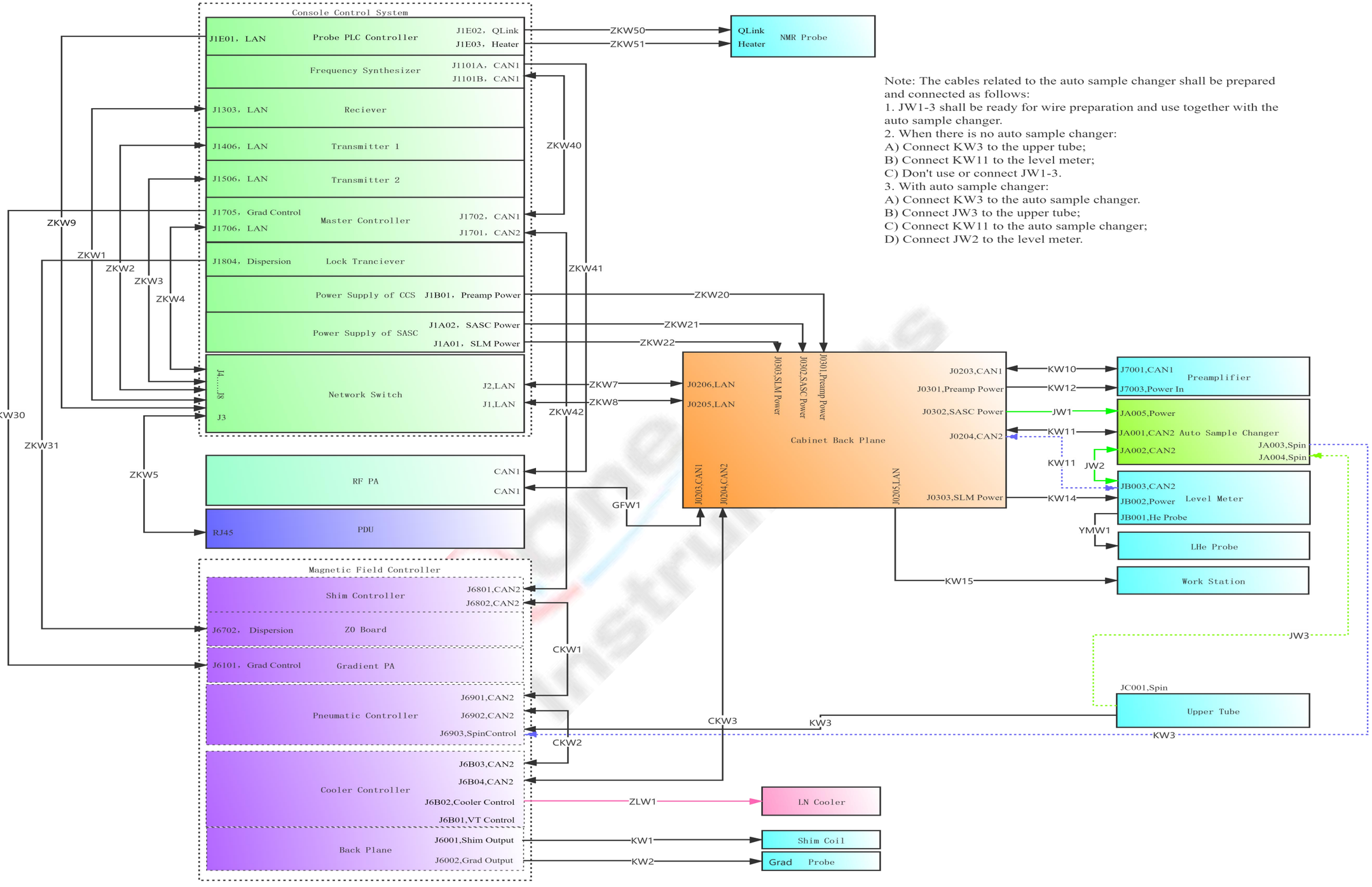


Fig. 15 2 Channel System Cabinet External RF Cable Connection Diagram



Note: The cables related to the auto sample changer shall be prepared and connected as follows:
1. JW1-3 shall be ready for wire preparation and use together with the auto sample changer.
2. When there is no auto sample changer:
A) Connect KW3 to the upper tube;
B) Connect KW11 to the level meter;
C) Don't use or connect JW1-3.
3. With auto sample changer:
A) Connect KW3 to the auto sample changer.
B) Connect JW3 to the upper tube;
C) Connect KW11 to the auto sample changer;
D) Connect JW2 to the level meter.

Fig. 16 2-Channel System Signal Cable Connection Diagram

The initial installation of the cables are completed by Q.One installation engineer. You only need to check whether the connector is connected reliably regularly during use. All signal cables of Quantum-I ^{Plus} NMR spectrometer use self-locking plugs, which will not loosen after insertion. Radio frequency cables use threaded joints and are tightened with torque wrenches during installation, which will not loosen under normal circumstances. However, you should check regularly to prevent radio frequency radiation and signal attenuation that may be caused by loosening of radio frequency connectors.

2.5 Software Installation

SpinStudioJ software can directly run executable files. The installation steps are as follows:

1) Copy the Q.One NMR compression package from the installation disc to the installation destination.
2) Decompress the compressed packet to local.
3) Send the folder's executable shortcut to the desktop.
4) Double-click the icon on the desktop to run SpinStudioJ.

SpinStudioJ needs to set spectrometer parameters after operation, which is carried out by Q.One installation engineer. If you need to set parameters, please check the SpinStudioJ User Manual, and if you have any questions, please consult Q.One.

3 System Operation

In general, before using Quantum-I ^{Plus} NMR spectrometer for nuclear magnetic resonance experiments and during the daily maintenance of the spectrometer, you need to do the following work to ensure the normal operation of the spectrometer:

- Power on: that is, turn on the power supply switches of each component of Quantum-I ^{Plus} NMR spectrometer, including checking the power supply, replacing fuses, etc.
- Check the working status of the system: The hardware system of Quantum-I ^{Plus} NMR spectrometer is equipped with detailed working status indicator lights. You can easily judge the working status of each component by whether there is a red light display.
- Manual operation: When using Quantum-I ^{Plus} NMR spectrometer, some tasks need to be manually operated by you, such as switching the power supply of various systems, replacing filters, etc. Not all manual operations are necessary, but you are required to perform these manual operations under certain circumstances.

3.1 System Operating Conditions

NMR spectrometer system is a kind of precision spectrometer equipment. Changes in external environment will significantly change the performance of the system (such as sensitivity, stability, etc.). Therefore, it is very important to ensure the conditions for the system to operate.

3.1.1 Power supply

NMR spectrometer shall be equipped with UPS power supply with voltage stabilizing function. UPS shall provide rated load power of at least 3KW and battery capacity shall not be less than 800AH.

3.1.2 Dedicated ground wire

In order to reduce electromagnetic interference and reduce the failure rate of NMR

spectrometer, it is necessary to provide a special ground wire for NMR spectrometer. The special ground wire needs to be separated from the zero line (the ground wire may be misconnected into the zero line, and when the load is unbalanced, the zero line is charged).

Special ground wire system shall be constructed by professional ground wire unit to ensure quality. After construction, special equipment shall be used to measure grounding resistance, and the measured grounding resistance shall be ≤ 4Ω. The special ground wire is introduced into the laboratory by using low resistance copper strip, and the strip at the laboratory end is drilled, which is convenient to fix the ground wire of the nuclear magnetic resonance spectrometer with bolts.

Special ground wire is connected to the shell of control cabinet, magnet and other components of the NMR spectrometer. During use, attention should be paid to check whether it is loose or disconnected.

3.1.3 Temperature and humidity

The following table lists the control requirements for the laboratory temperature range, temperature change speed and humidity. In addition, the temperature near the magnet cannot change rapidly. If the room temperature fluctuates rapidly during the experiment and shimming, the uniformity of the magnetic field will be greatly affected.

The temperature fluctuation in the laboratory should be controlled within the range of less than 1 ℃/hour. If the altitude is too high (over 1500 meters), the temperature requirement can be relaxed by 1 ~ 2 ℃. The laboratory shall be equipped with an air conditioner with sufficient power to control the indoor temperature and a dehumidifier to control the indoor humidity.

Be careful not to let sunlight directly shine on the magnet and its nearby positions, and the air outlets of air conditioners and dehumidifiers should not face the magnet.

Air conditioning should also be installed in the air compressor room to prevent the air compressor from being damaged due to overheating.

Table 3 Temperature and Humidity Control Requirements

	Temperature/℃	Temperature/° F	Relative humidity
Available Range	17-24	60 ~ 75	20 to 80 percent
Optimum value	20	68	40%-60%
Stability Requirements	± 1.0	± 1.8	
Unavailable Range	-20 ~ 60	-4 ~ 140	8%~80%t

3.1.4 Ground vibration

Ground vibration with a certain intensity and frequency will generate interference signals on the spectrum, and the stronger the magnetic field, the more sensitive the spectrometer is to the vibration. Therefore, the floor should have sufficient strength to reduce the adjacent dynamic vibration to a negligible level, requiring the single peak intensity of ground vibration to be no more than 20ug and the vibration frequency to be less than 100Hz.

It should be noted that during the use of NMR spectrometer, large compressors, generators, central air conditioners and other mechanical equipment should not be installed in the adjacent areas. At the same time, it should continuously monitor whether the ground vibration meets the requirements. If the vibration exceeds the allowable range, open the air source input of the vibration isolation column to keep the magnet in a suspended state. If the experiment is stopped for a long time, the air source of the vibration isolation column can be turned off.

3.1.5 Magnetic field environment

Under the confirmation of Q.One installation engineer, the environmental magnetic field conditions of the installation site should have been met, but during the use of the spectrometer, new changes may inevitably occur around the spectrometer, such as the installation of new equipment and the construction of new roads. The following is specified in the Installation Preparation Manual for Quantum-I *Plus* NMR Spectrometer, and the important contents are listed here as necessary supplements.

Common sources of magnetic field interference include dynamic load power lines, radio

frequency or television base stations, high-power transformers, motors and similar electromagnetic equipment. Please keep the magnet at least 4.6 meters away from strong electromagnetic equipment, electric motors, electric forklifts, etc.

Similarly, the magnet is kept at the same distance from any other object that may adversely affect the uniformity or integrity of the magnetic field. Objects that may affect the magnetic field include (but are not limited to): walls covered with metal skins or embedded with steel bars, reinforced concrete structures, storage rooms for iron equipment, etc. The environmental changes of the system site should be carefully analyzed to ensure that the magnets can work in the best condition. Table 6 lists the interaction between common objects and magnetic fields.

WARNING *Cardiac pacemaker carriers can only approach the magnet unless your safety can be reliably guaranteed, otherwise please keep a distance of more than 4.5 meters from any direction of the magnet. The strong magnetic field generated by superconducting magnets will affect the work of cardiac pacemakers and may bring death or other serious risks. Please consult the user's manual of cardiac pacemaker, contact the manufacturer of cardiac pacemaker, or consult a doctor to confirm the harm of magnetic field to cardiac pacemaker. Q.One has equipped each system with a warning sign to warn of the danger of cardiac pacemakers. Please place the prompt sign 4.5 meters away from the magnet.*

Table 4 Interaction of Magnetic Fields between Objects and Magnet

Objects affect the magnetic field of a magnet	
Above 15 Gauss	All ferromagnetic objects, except a small number of objects not exceeding 11kg per square meter.
5-15 Gauss	Moving or fixed ferromagnetic objects above 45kg, such as trolleys, gas tanks, etc.
2-5 Gauss	Moving or fixed ferromagnetic objects above 450kg, such as pickup trucks, automobiles, flatbed trucks, electric forklifts, elevators, etc.
1-2 Gauss	More than 34000kg of moving or fixed ferromagnetic objects, such as trains, trucks, etc.
Objects affected by the magnetic field of a magnet	

Above 15 Gauss	Heart pacemakers, ferromagnetic prostheses (or other implants), unfixed ferromagnetic objects, such as tools, keys, electronic devices, watches, magnetic storage media, credit cards, etc.
5-15 Gauss	Cardiac pacemaker, electronic equipment, such as CRT display, computer, projector, etc.
2-5 Gauss	High sensitivity electronic equipment, such as unshielded projectors, etc.
1-2 Gauss	High sensitivity electronic equipment, such as linear accelerator, electron microscope, CRT display, etc.

The peak-to-peak value of electromagnetic interference in NMR spectrometer laboratory should be less than 5 milligauss. During the use of the spectrometer, in addition to control the objects that interact with the magnet to approach the magnet, for uncontrollable objects such as trains, trucks and elevators, the laboratory must be kept at a sufficient distance from them. NMR laboratory administrators should pay attention to possible changes around the laboratory and maintain communication with relevant departments such as water and electricity installation, urban planning, urban construction, etc. to ensure that these items will not appear within the safe distance of the system. The minimum distance requirements for some typical interference sources from the magnet are shown in the following table.

Table 5 Minimum Distance Requirements for Typical Electromagnetic Interference from Magnet

Interference source	Minimum distance from magnet requirement
Subway, tram	250m
Elevator, electric forklift	10m
Magnetic field abrupt mass spectrometer	30m

3.1.6 Ferromagnetic objects

There should be no ferromagnetic objects within the 5 Gauss line range of the magnet, and there should be no ferromagnetic objects weighing more than 250Kg within the 1 Gauss line range.

If the laboratory is on the first floor and the building has an underground garage, the lower part of the laboratory should be closed to ensure that no cars can pass under the magnet.

Taking the center line of the magnetic field as a reference, the ranges of 5 Gauss lines

and 1 Gauss lines for different types of magnets are shown in the following table.

Table 6 Magnet 5 Gaussian Line and 1 Gaussian Line Range

Magnet	Horizontal 5 Gauss Line (m)	Vertical 5 Gauss Line (m)
AS400	1.00	2.8
AS600	1.60	4.5

3.2 Power on

The Quantum-I *Plus* NMR spectrometer control cabinet and NMR workstation need to be powered on manually, and the two can be turned on separately regardless of sequence. In principle, NMR workstations and consoles should be in a long-term operation state, and power supply should not be cut off except for power failure and maintenance.

WARNING *It is strictly prohibited to switch the power supply of NMR control cabinet and NMR workstation frequently to ensure that the interval between shutdown and startup is not less than 1 minute.*

Frequently shutdown (i.e. The interval between shutdown and startup is not more than 1 minute) may cause hardware damage to NMR console, and components may not work or work in the wrong state after damage, and even further cause damage to connected components. The general requirement is to restart the spectrometer at an interval of more than 1 minute after shutdown. Although the computer hardware system used by NMR workstations is relatively mature, the operating system may still be damaged. When the system is confirmed to be damaged, please immediately turn off the power supply and contact Q.One.

3.2.1 Turn on the NMR workstation

Turn on the workstation computer and monitor, and the workstation will start and enter the operating system interface.

After the system starts, double-click the icon on the desktop to start SpinStudioJ. After

startup, the software interface is shown in the following figure. If the main control system of the control cabinet is turned on and running normally, the spectrometer status at the bottom right will be displayed as "idle". If SpinStudioJ cannot connect to the master system, the information prompt bar will display a connection error message.

The standard console control system includes: receiver, 2 transmitters, main control board, field lock board and clock board. The receiver, transmitter and main control board are all located in 192.168. 5. X network segment, and the corresponding IP address terminal segments are respectively: receiver 24, broadband transmitter 23, high band transmitter 22 and main controller 21. If the connection fails, you can judge the failure point through IP to facilitate Q.One to carry out maintenance.

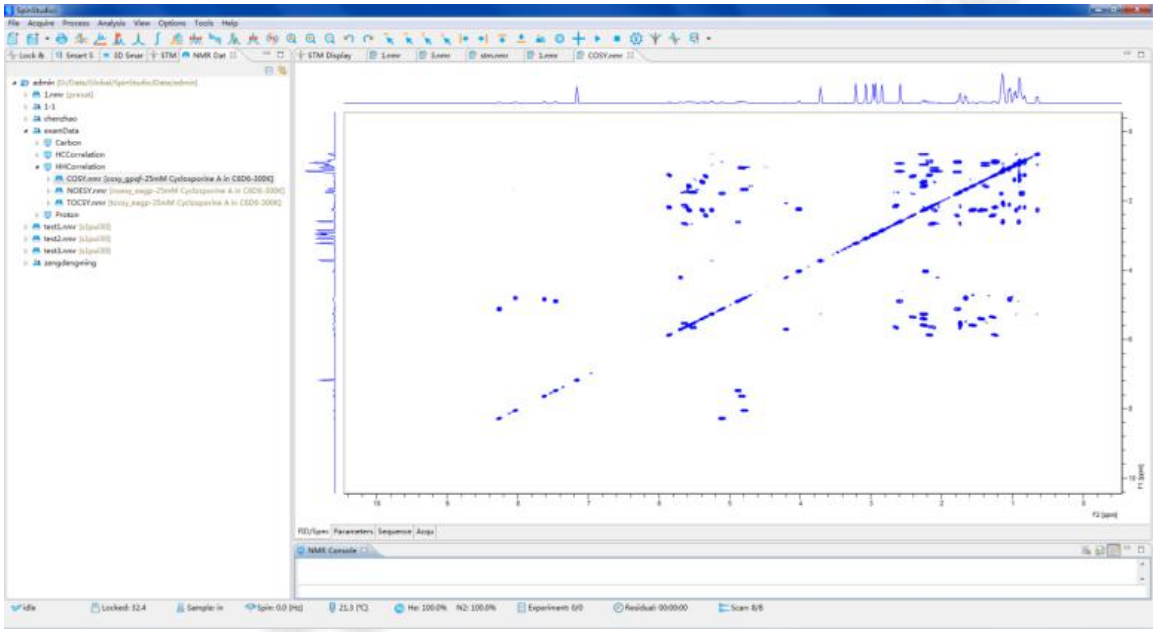


Fig. 17 SpinStudioJ Software Interface

3.2.2 Turn on the NMR console

The power switches of each subsystem in the Quantum-I *Plus* NMR spectrometer control cabinet are located on the right side of the rear of the chassis. When turning on or off, you can choose to manually turn on or off all switches one by one.

- Main power switch: located at the bottom of the rear of the cabinet, it will be turned on when the air switch is turned upwards, and PDU will display the current power supply

voltage at the same time.

The main power switch is equipped with an undervoltage protector. When the voltage is insufficient, the air switch will be automatically cut off and can only be recovered manually.

- Three-in-one power switch of magnetic field control system: located at the top right of the rear panel of the chassis. After the power switch is turned on, the power indicator of the switch will light up. A delay fuse is installed inside the three-in-one switch. When the current exceeds the limit value, the fuse will blow to avoid damage to the internal circuit.
- RF power amplifier three-in-one switch: located at the top right of the rear panel of the chassis, the switch is turned on when the switch is pressed to make "O" upward.
- Three-in-one power switch of the main control system: located at the lower right of the rear panel of the chassis. After the power switch is turned on, the power indicator of the switch will light up. A delay fuse is installed inside the three-in-one switch. When the current exceeds the limit, the fuse will blow to avoid damage to the internal circuit.
- The power switch of the front playback system is located on the rear panel of the main control system. When the torsion switch is turned to the right in the direction indicated by the "Enable" arrow, the power of the front playback system will be turned on, and the 7.5 V, 15V and-15V power indicator lights above will be turned on at the same time.
- Injector power switch: located in the rear panel of the main control system, when the torsion switch is turned to the right in the direction indicated by the "Enable" arrow, the injector power supply is turned on.
- Liquid level gauge power switch: located on the rear panel of the main control system, when the torsion switch is turned to the right in the direction indicated by the "Enable" arrow, the liquid level gauge power supply is turned on.
- Probe power switch: located in the rear panel of the main control system. When the torsion switch is turned to the right in the direction indicated by the "Enable" arrow, the probe power is turned on and the + 24V power indicator above will be lit.

3.3 System startup status check

3.3.1 Startup Status of Console Control System

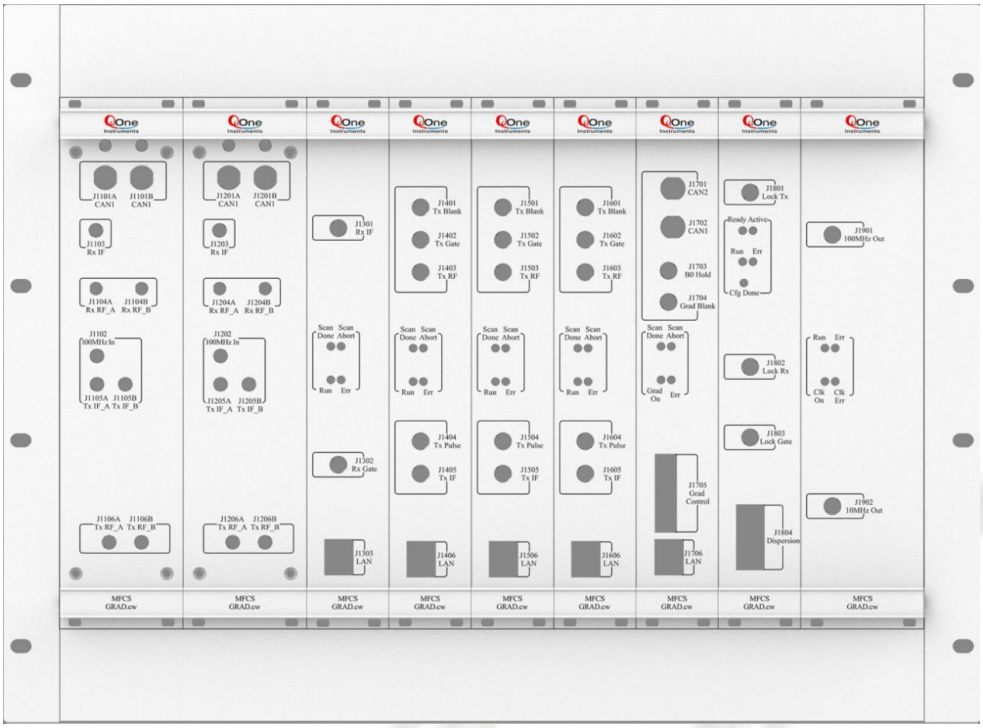


Fig. 18 Distribution of LED in front panel of console control system

The distribution of status indicator lights on the front panel of the main control system is shown in the figure. Under normal starting, normal working and wrong states, the status of each indicator light is as follows:

Table 7 LED Display Status of Front Panel of Main Control System

Serial Number	Identification	LED Color	LED Meaning	Normal startup state
1	A Act	G	Frequency Configuration Activity	Flip after each receive
2	B Act	G	Frequency Configuration Activity	Flip after each receive
3	Scan Done	G	Pulse Sequence Execution Completed	It is normally bright and goes out during sampling.
4	Run	G	The FPGA configuration of that receive is successful, and the system starts up normally	Flicker
5	Scan Abort	R	Receiver FPGA configuration	Extinguish

Serial Number	Identification	LED Color	LED Meaning	Normal startup state
			failed	
6	Err	R	Receiver Start Error	Extinguish
7	Scan Done	G	Pulse Sequence Execution Completed	Normally bright, extinguished when broadband sampling
8	Run	G	Wideband Transmitter FPGA Configuration Successfully	Chang Liang
9	Scan Abort	R	Sampling Error	Extinguish
10	Err	R	Wideband Transmitter FPGA Configuration Failed	Extinguish
11	Scan Done	G	Pulse Sequence Execution Completed	Normally bright, extinguished when high band sampling
12	Run	G	High Band Transmitter FPGA Configuration Successfully	Chang Liang
13	Scan Abort	R	Sampling Error	Extinguish
14	Err	R	High Band Transmitter FPGA Configuration Failed	Extinguish
15	Scan Done	G	Pulse Sequence Execution Completed	Chang Liang
16	Grad On	G	Gradient work indication	Extinguish, light up when gradient works
17	Scan Abort	R	Pulse execution stop	Extinguish
18	Err	R	Gradient configuration failed	Extinguish
19	Ready	G	Fieldlock plate starts normally	Chang Liang
20	Err	R	Lock-up board data transmission in progress	Flicker
21	Run	G	The lockboard PLL is locked	Chang Liang
22	Err	R	Communication Error	Extinguish
23	Run	G	Clock Board Operation Indication	Chang Liang
24	Err	R	Clock board operation error	Normal extinction
25	ClkOn	G	Clock Board Clock Normal Output	Always bright, mistakes often go out.
26	ClkErr	R	Clock Board Clock Output Error	Often go out, mistakes often light up.

3.3.2 Start-up Status of RF Power Amplifier

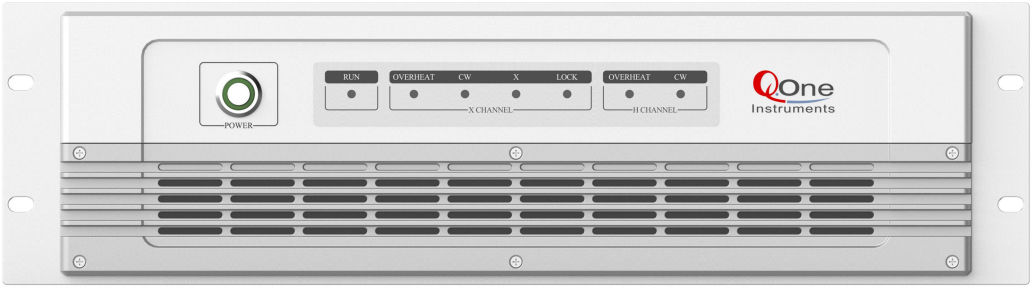


Fig. 19 RF Power Amplifier Indicator Lamp

Power: red or green color light, which indicate the power supply status of the power amplifier controller. After the AC current is turned on, the lamp is on.

RUN: Green indicates that the system is normal, and red indicates that the system is in bypass mode (not working), with red or green flashing.

CW: Yellow light, which indicates that the power amplifier works in continuous wave mode when lit. The lamp shall be normally off.

OverHeat: Red light, which indicates that the power amplifier is in an over-heated state when lit. Under normal conditions, the lamp should be turned off normally.

WARNING *When any red indicator light of the RF power amplifier is lit, please immediately stop transmitting pulses. Continuous overheat may cause the power amplifier to burn down.*

3.3.3 Starting State of Magnetic Field Control System

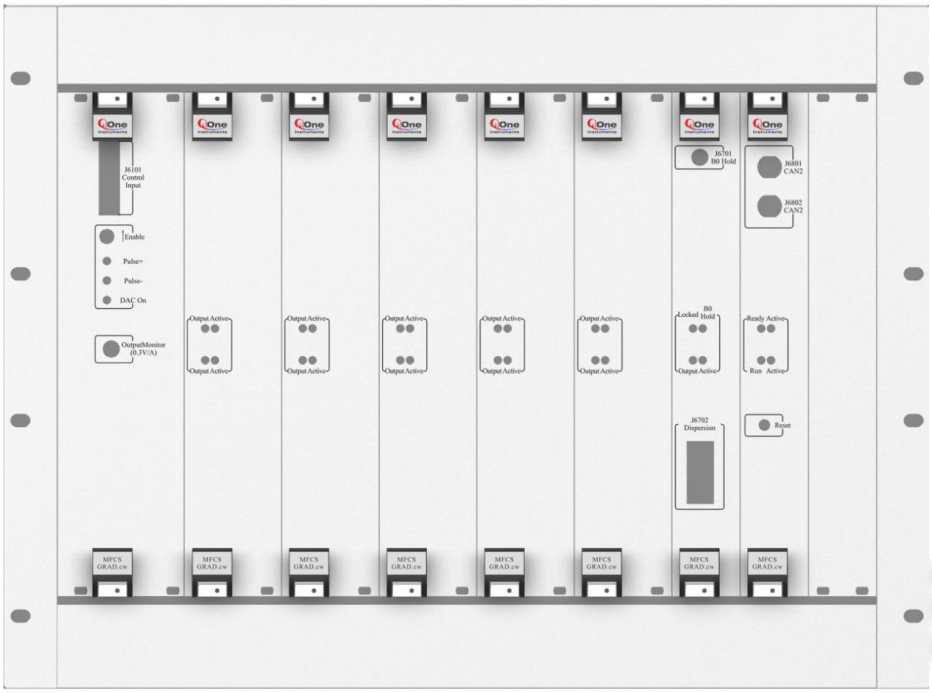


Fig. 20 Distribution of LED in Front Panel of Magnetic Field Control System

The indicator lamps of all channel boards are the same, and the LED number of only one channel board is marked as an example in the above figure.

When the system is started, the shim system will carry out self-inspection. The red LEDs of channel plates 6 and 7 and Z0 plates 10 and 11 will be lit for 1 second and all will be extinguished for 1 second. The green LEDs of channel board 4, 5 and Z0 board 8 are lit for 1 second and then extinguished.

The startup status of each LED is shown in the following table:

Table 8 Definition of LED Status of Front Panel of Magnetic Field Regulation System

Number	Identification	LED Color	Meaning	Normal startup state
1	Run	Green	Gradient power amplifier board configuration	Always on
2	Pulse +	Orange	Output positive pulse	Off, positive pulse output lights on
3	Pulse-	Orange	Output negative pulses	Off, negative pulse output lights on
4	Output	G	Either of the first four channels on the channel	Off, Lite when output

Number	Identification	LED Color	Meaning	Normal startup state
			board has an output	
5	Output	G	Either of the four channels behind the channel board has an output	Off, Lite when output
6	Err	R	Output error in any of the first 4 channels on the channel board	Extinguish
7	Err	R	Output error in any of the last 4 channels	Extinguish
8	Locked	G	Field Lock Indicator	Off, lit when the lock level is above the threshold
9	Z0 Output	G	Channel Z0 Output	Off, Z0 lights up when it has output
10	B0 hold	Red LED	B0 hold signal indication	Turn off B0 hold Valid Lighting
11	Z0 Err	Red LED	Channel Z0 Output Error	Off, Z0 output illuminates abnormally
12	Ready	Green LED	Control panel ARM starts normally	On
13	Active	Red LED	CAN transceiver data	Normally extinguished, flashing when receiving and receiving data
14	Run	Green LED	FPGA start up normally	On
15	Err	Red LED	FPGA startup failure	Extinguish

3.3.4 Start-up Status of Preamplifier

Fig. 21 Preamplifier System Display Screen

When the system starts, the display screen displays the following status:

(1) The installed front layer is displayed in the display screen and the status is Ready.

(2) The CAN communication status is indicated as normal.

3.4 Manual Operation

3.4.1 Reset switch

The control board of the magnetic field control system is equipped with an external reset switch, and the corresponding controller can be reset to the startup state by pressing the reset switch for more than 1 second. The reset switches are all trapped in the panel to avoid accidents caused by false triggering of reset. When reset, please insert the reset thimble into the reset hole and press and hold the reset key for more than 1 second.

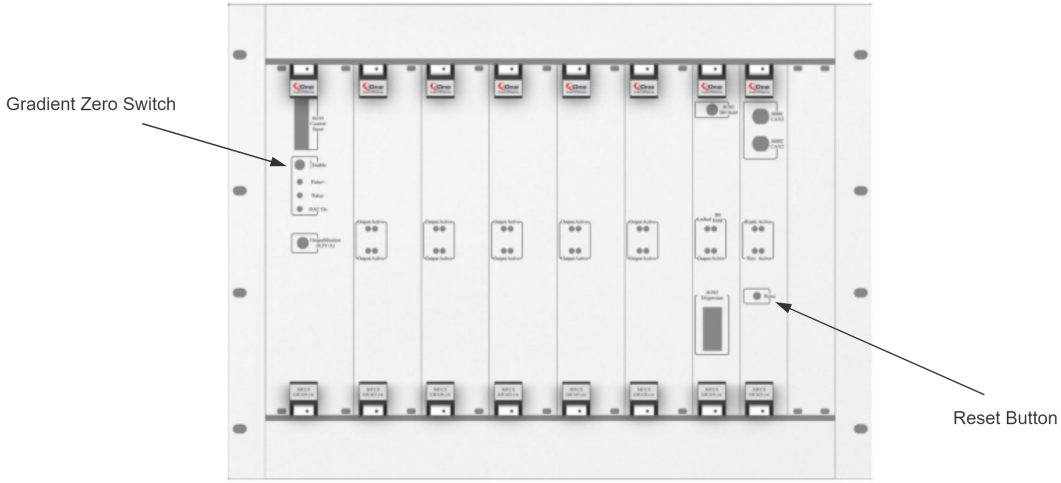


Fig. 22 Location Diagram of Reset Switch of Magnetic Field Regulation System

As shown in the above figure, the reset of the magnetic field control system includes the communication reset of the gradient power amplifier and the shim system. The gradient reset switch is located in the middle of the front panel of the gradient power amplifier board. After reset, the gradient pulse being output will be immediately suspended and enter an idle state. The shimming system communication reset switch is located in the middle and lower part of the front panel of the control panel. After reset, the communication system will restart, but the control and output of the shimming system will not be affected.

3.4.2 Change RF filter

Quantum-I *Plus* NMR Spectrometer is equipped with broadband high-pass or low-pass filters. Generally, the filter does not need to be replaced. By default Q.One installation engineer will give priority to your most commonly used configuration when installing the filter. When necessary, you can change the filter according to the following rules:

- The lock channel standard is equipped with D nucleus band-pass filter. If F-lock is needed, please change the filter with F-band-pass filter.
- High band channel: ^{1}H high pass and ^{1}H-^{19}F high pass filters:
  a. When you need to carry out ^{1}H and ^{19}F related experiments, replace the high band filter with ^{1}H high power filter.

b. When you need to detect ^{1}H or ^{19}F, or need to carry out X-observe and ^{1}H or ^{19}F decoupling experiments, replace the high-band filter with an H-F high-pass filter.

- X Channel: When you need to transmit ^{19}F nucleus on the broadband channel, change the X low-pass filter with an X-F filter, otherwise replace it with an X filter.

3.4.3 Tuning

The Quantum-I ^{Plus} NMR spectrometer is equipped with a manual probe or an automatic STM probe. If an automatic STM probe is provided, please ignore the contents of this section. If a manual probe is provided, please tune as follows:

(1) Put in the experimental sample.

(2) Open the tuning window in SpinStudioJ software and select the tuning core.

(3) Click the "Start Tuning" button to start tuning.

(4) Alternately adjust the tuning and matching twist on the probe so that the lowest point of the tuning curve is located at the tuning frequency point and the minimum value is minimized.

(5) Click the "Stop Tuning" button to stop tuning.

3.4.4 Switching of Gradient Power Amplifier Zero Switch

The shift switch (labled as Zero) at the top of the front panel of the gradient power amplifier is used to switch the process zero of output static current enable state of the gradient, if the switch is switched to the direction of the arrow, the zero process starts. In the disabled state, the gradient power amplifier will output pulses but with non-zero static current output. When zero process is finished, the zero LED light lit on.

By default, the zero switch should always be switched to the on state. It will automatically start the zero process at power on if the switch is on.

3.4.5 Monitoring of Gradient Power Amplifier Output Pulse

The Output Monitor SMA connector on the gradient power amplifier panel is used to

monitor the output pulse of the gradient power amplifier. Connect it to the oscilloscope with coaxial line. Set the impedance of the oscilloscope to a high impedance mode, and adjust the scanning time to be greater than the positive and negative pulse width time. Then the pulse signal output of the gradient power amplifier can be captured by a single trigger mode.

The gradient power amplifier outputs a 1:1 potential voltage corresponding to the output current, one ampere current outputs, 1V voltage can be monitored at the monitor port.

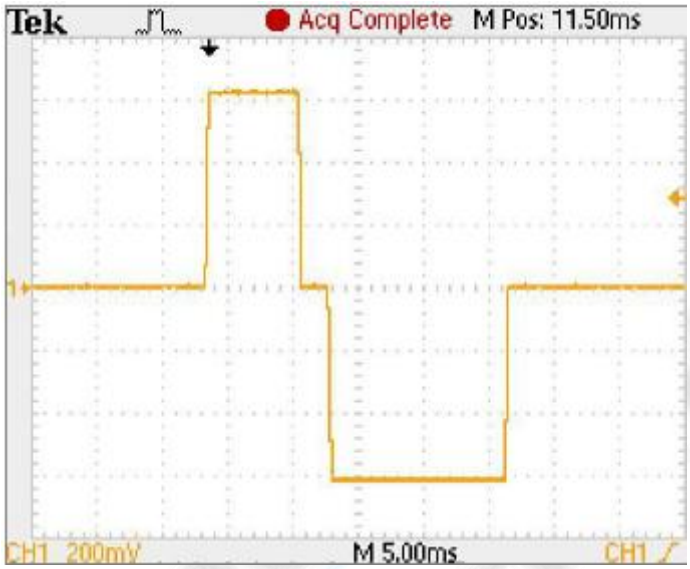


Fig. 23 Gradient Output Pulse

If the gradient experiment cannot be carried out, you can try to monitor the output state of the gradient amplifier via the monitor connector. If you do not have oscilloscope, please contact Q.One.

3.4.6 Switching of Z0 Output Direction

The switch S1 on Z0 board is used to control the current output direction of Z0 channel of shim power supply. If the current direction of Z0 channel is correct, the lock level will rise due to normal lock feedback after lock on, and the lock error line and the lock level line will remain parallel. If the current direction of Z0 channel is wrong, the lock level line will twist into a curve shape due to wrong lock feedback after the field is locked on. At this time, the current direction of Z0 channel needs to be changed. The switching method is to turn the switch S1 of Z0 board to the opposite direction.

The position of Z0 board in the magnetic field control system is shown in the following figure:

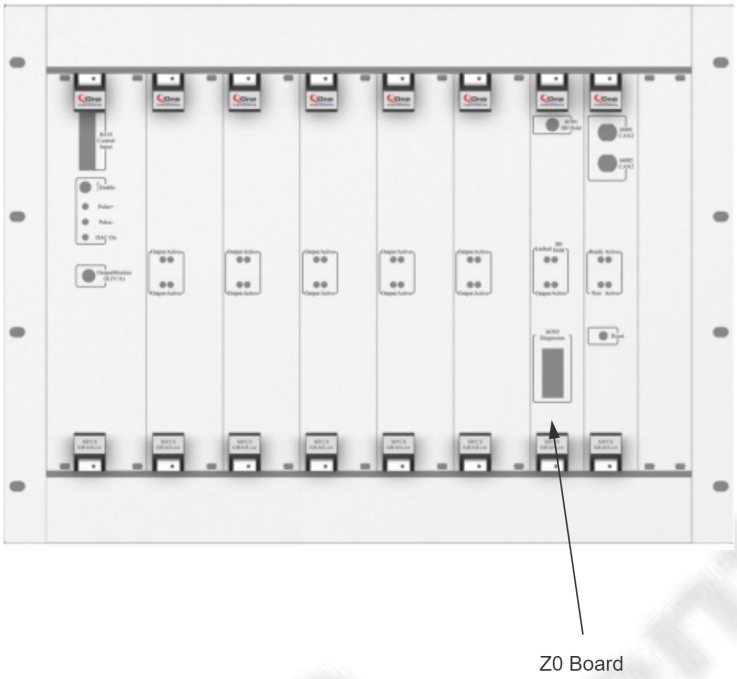


Fig. 24 Position of Z0 Board in Magnetic Field Control System

After removing the Z0 channel circuit board, turn switch S1 in the opposite direction. The position of switch S1 on the Z0 board is shown in the figure:

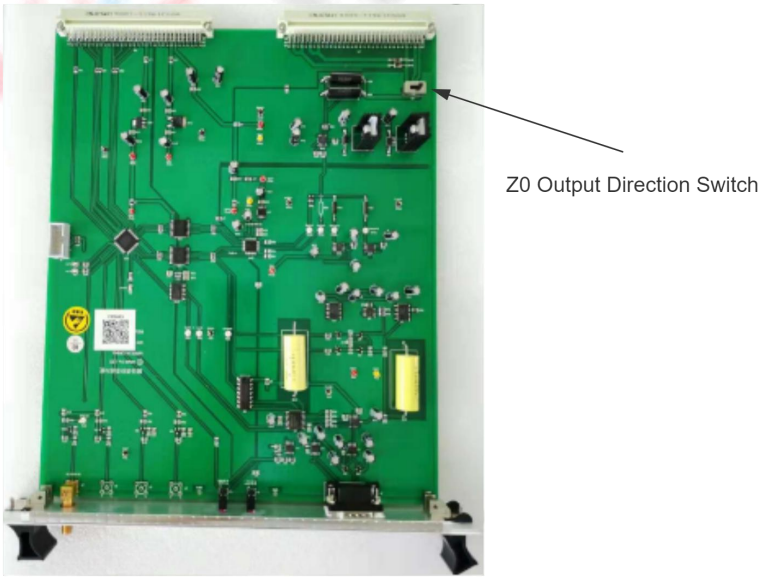


Fig. 25 Position of switch S1 on the Z0 board

After installation and testing, switch S1 of Z0 board has been set to the correct direction, and you do not need to make any changes. This switch can only be turned when Z0 output is reversed due to replacement of shim coil or magnet.

3.5 Shutdown the Spectrometer

There is no special requirement for the shutdown of superconducting NMR spectrometer. Just turn off the power switches of each system in the control cabinet one by one in any order, and finally turn off the main power switch behind and below the control cabinet.

When turning off the spectrometer, please turn off the switch on the front panel of the power amplifier, the turn the switches of the automatic sample changer and the switch of the liquid level meter at the back of the console control system to the opposite direction of the arrow to turn off the corresponding power supply.

CAUTION *After turning off the main power switch of the control cabinet, when the main power socket of the control cabinet is not unplugged, the input end of the main power air switch of the control cabinet is still charged. If you need to operate the cabinet adapter board behind the control cabinet, please turn off the input switch of the main power first or unplug the main input power cable of the cabinet!*

CAUTION *In order to avoid excessive surge impact during power on, please turn off the power switches of all systems at first when turning off the power supply of the control cabinet. It is forbidden to turn off the main power switch of the control cabinet and keep the power switch of each system on!*

3.6 Replace fuses

If the indicator light of the power switch is not lighted when the input power of the control cabinet is normal and the system power switch is turned on, the fuse in the power switch needs to be replaced. The replacement steps are as follows:

1）Unplug the AC power input cable of the system.

2) Use a flat screwdriver to gently pry out the fuse installation box from the middle of the socket (there is a fuse mark on it):

3）Pull out the fuse installation box, remove the fuse and install a new fuse.

4）Push in the fuse box, plug in the power cord and power on.

4 Run NMR experiments using Quantum-I *Plus* NMR spectrometer

4.1 Samples

4.1.1 Requirements for samples

The sample for structural test should be pure single component. The sample for high resolution spectrum shall be a substance that has appropriate solubility to the solvent to be determined and does not react with the solvent (except for those who specifically react). The prepared sample solution should have good fluidity (except for polymers). There should be no suspended solid particles in the sample solution, especially no ferromagnetic dirt, and the use of high concentration salt substances should be avoided as much as possible.

The prepared sample solution shall have sufficient volume, the sample volume in the 5mm sample tube shall not be less than 0.45 ml, and the sample volume in the 10mm sample tube shall not be less than 1.8 ml. For samples requiring special tests, they can be considered comprehensively according to the specific test contents and the above requirements. The solution of the sample should have a low viscosity, otherwise the resolution of the spectral peak will be reduced. The sample dosage should ensure the necessary signal-to-noise ratio.

The outside of the NMR sample tube shall be clean, There should be no pollutants such as solution and impurities outside the NMR tube. Although the slight dirt of a single NMR tube is not enough to affect the test results, it will lead to the gradual accumulation of probe pollutants and eventually lead to all data tested by the spectrometer carrying various pollutant interference signals, affecting the judgment of the accuracy of the test results.

4.1.2 Sample solvent and reference

During the internal locking test, the sample is dissolved in deuterated reagent. Deuterated reagents often contain reference substances for the nuclei measured in the sample (i.e. Used as a reference for calibrating chemical shifts). See Table 13 for the chemical shift values and multiplicity of spectral lines of commonly used references for ^{1}H and ^{13}C spectra.

Table 9 Deuterated Solvents Commonly Used in NMR Experiments

Name	Molecular formula	^{1}H (ppm)	Multiplicity	^{13}C (ppm)	Multiplicity
Deuterated acetone	CD3COCD3	2.04	5	206 29.8	(13) 7
Deuterated benzene	C6D6	7.15	1 (Width)	128.0	3
Deuterated chloroform	CDCL3	7.24	1	77.0	3
Heavy water	D2O	4.60	1	-	-
Deuterated dimethyl sulfoxide	CD3SOCD3	2.49	5	39.5	7
Deuterated methanol	CD3OD	4.78	1	49.0	7
Deuterated dichloromethane	CD2CL2	5.32	3	53.8	5
Deuterated pyridine	C5D5N	8.71 7.55 7.19	1 (Width) 1 (Width) 1 (Width)	149.9 135.5 123.3	3 3 3

4.1.3 External Lock Method

When working in an external locking mode, the solvent should generally contain no nucleus to be tested, and the liquid sample can be directly used as a sample. The reference substance is not completely mixed with the sample. Usually, the reference substance is packaged in a capillary tube and put into the sample to be tested for simultaneous testing. If necessary, the measured value is corrected according to the volume susceptibility. Correction formula is:

$$\delta_1 = \delta_0 + (\chi_1-\chi_2)\, 2\pi/3 \qquad \text{(Equation 1)}$$

Where:

δ_1—corrected chemical shift value.

δ_0—observed chemical shift value.

χ_1—volume susceptibility of the sample.

χ_2—Volume susceptibility of reference material.

4.1.4 Sample preparation

Use sample solution or liquid sample with appropriate concentration, including internal standard or external standard, and there should be no insoluble substances and bubbles in the sample solution. The peak height of the reference substance in the spectrum should not be too strong. For samples requiring precise testing (such as measuring relaxation time), oxygen removal can be carried out by "cyclic freezing method" as required.

4.1.5 Determination of Sample Location with Gauges

In NMR experiment, the test solution part of the sample tube should be in the center of the probe coil, and the sample position can be conveniently determined by using the sample rack provided by Q.One, as shown in the following figure.

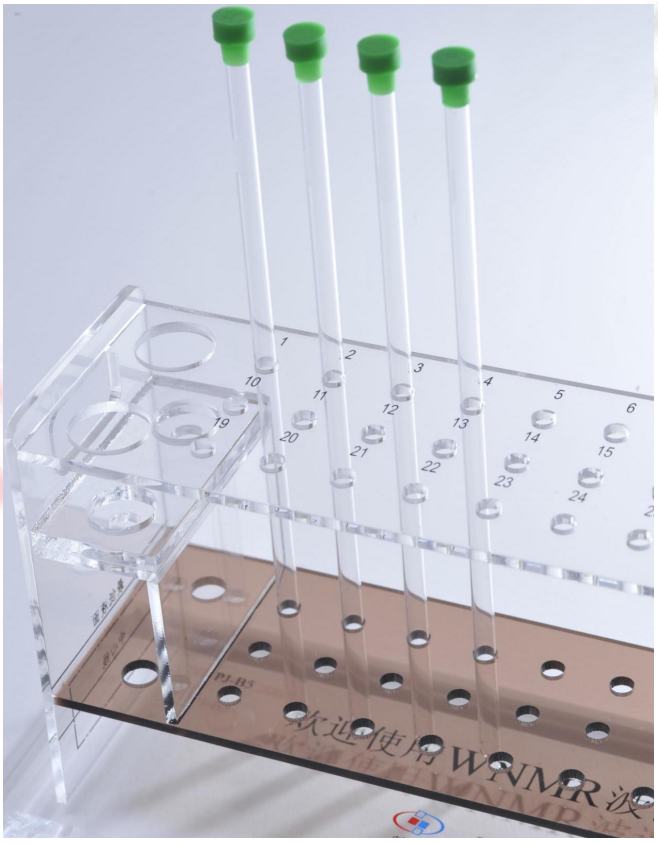


Fig. 26 Gauges, Samples

Insert the sample tube into the rotor, then put the rotor into the rotor hole of the sample rack, and insert the sample tube to the bottom. The lowest height of the sample should exceed

the height of the dark partition plate.

4.2 Run NMR Experiments

4.2.1 Use SpinStudioJ

SpinStudioJ, the software for controlling and data processing the Quantum-I^{Plus} NMR spectrometer, provides an operating interface for controlling the Quantum-I^{Plus} NMR spectrometer, displaying the running status and experimental results of the spectrometer.

All operations can be carried out through the graphical interface and the command line. The running status and experimental results of the spectrometer can be displayed through the graphical interface or directly viewed through the command line.

The "SpinStudioJ Operation Manual" describes the steps and methods of using SpinStudioJ in detail, while the "SpinStudioJ Command and Parameter Manual" describes the commands and their usage in detail.

4.2.2 Use appropriate pulse sequence parameters

The purpose of using appropriate pulse sequence parameters is to obtain better experimental results, but it also includes selecting appropriate experimental parameters to obtain correct experimental results. SpinStudioJ's simple single pulse sequence is shown in the figure.

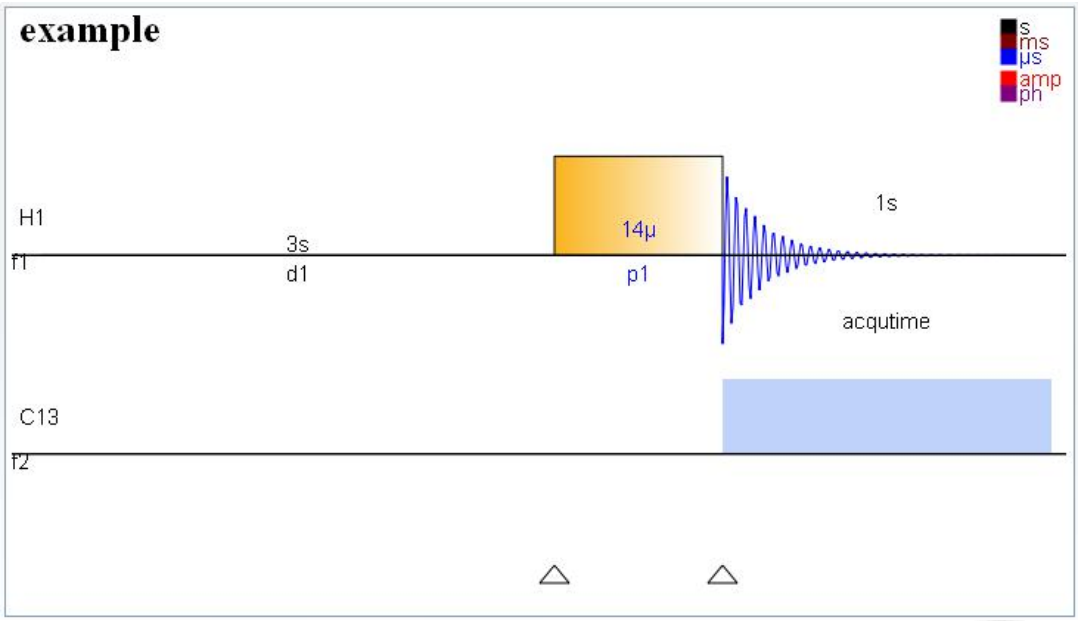


Fig. 27 SpinStudioJ single pulse sequence

The main parameters in the pulse sequence include:

Nucleus 1: Launching nucleus (experimental channel)

Freqs1: Transmit Frequency in MHz

Plvl1: transmit power

Freqoff1hz: Transmit Frequency Offset in Hz

Swhz: Sampling Spectrum Width (in Hz)

Swppm: Sampling Spectrum Width (in ppm)

Fidpoints: Sampling points

Rxgain: Receive Gain

Ns: Number of scans

Dummyscans: number of empty scans

d1: Relaxation wait time (in seconds)

p1: Pulse width in microseconds

Acqutime: Sampling time in seconds

SpinStudioJ's command name is different from that of Varian and Bruker and requires

you to be familiar with it for a period of time, but at the same time all parameters can be entered through the parameter interface. The command line has prompts and auto-completion functions, and you can enter commands according to the prompts. If you have experience using Bruker or Varian NMR spectrometers, Appendix 1 provides SpinStudioJ and Bruker, Varian command and parameter reference tables to facilitate you to quickly understand the meaning and usage of SpinStudioJ commands and parameters.

To correctly obtain NMR signals, when creating any new experimental pulse sequence, special attention should be paid to the following contents:

(1) **Appropriate pulse transmission power**

The pulse transmission power plvl1 can be arbitrarily set from-30 to 63. When plvl1 = 63, the radio frequency transmission system outputs the pulse signal at the maximum power. However, due to the maximum linear transmission power of the radio frequency power amplifier, the larger the plvl1 value, the better. In general, the emission power linearity curve of Quantum-I Plus NMR spectrometer is shown in the following figure:

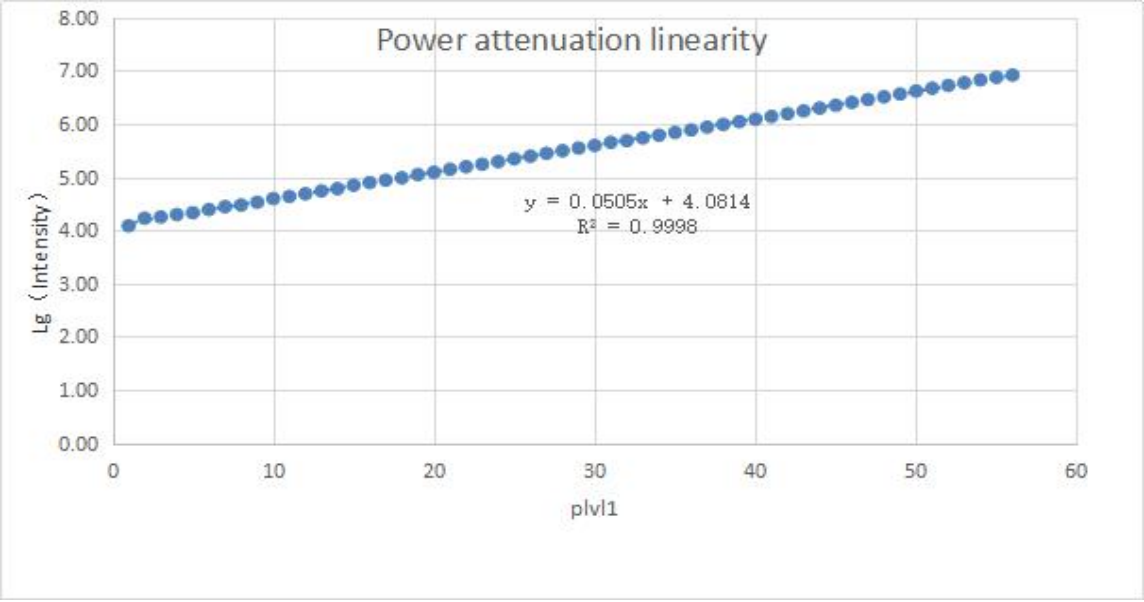


Fig. 28 Transmission Power Linear Curve of Quantum-I Plus NMR Spectrometer

When Plvl1 approaches the maximum value, the power of the transmitted signal tends to be saturated and the output power no longer increases linearly. The maximum transmitted

power value should be set according to the value of the most linear power, and the parameter may be slightly different for each NMR spectrometer. After the power amplifier is used for a long time, the power may decay. It is recommended to re-calibrate the power linearity regularly.

(2) **Appropriate gain**

SpinStudioJ supports automatic gain, which you can set automatically with the rga command.

If the gain is set manually, rxgain can be selected from 0 to 100, but too large rxgain will cause receiver overflow. In general, rxgain can be set slightly less than the overflow gain.

5 Operation and Maintenance Requirements

Nuclear magnetic resonance spectrometer is a precision large-scale spectrometer. The spectrometer should be checked and maintained frequently during use to ensure that the spectrometer works normally and in the best state. Improper usage or imperfect maintenance measures will lead to damage or shorten the service life of the spectrometer. If you have any questions during use and maintenance, please consult Q.One.

5.1 Magnet Maintenance

(1) Monitor the volatilization of liquid nitrogen and liquid helium every day and supplement liquid helium and liquid nitrogen on time.

The stock of liquid nitrogen and liquid helium can be read through SpinStudio. You can set the liquid level reading to automatic reading mode. The software will read the liquid level height regularly and form records. You can judge whether the volatilization rate of the liquid level is normal by recording the liquid level.

(2) Provide a constant temperature working environment for the magnet to prevent the magnet from being directly exposed to sunlight, so as to maintain the magnet in an ideal working state.

(3) The indoor temperature is kept in the range of 17 ℃ ~ 25 ℃, the temperature fluctuation speed is controlled to be less than 5 ℃/day and less than 1 ℃/hour, and the indoor humidity is in the range of 40% ~ 60%. Excessive temperature will lead to faster volatilization of liquid nitrogen and liquid helium and increase maintenance costs. However, too fast temperature change will seriously affect the stability of spectrometer performance, which is obviously shown in the experimental results.

(4) It is strictly prohibited for irrelevant personnel to enter the working area or approach the magnet.

(5) It is strictly prohibited to bring prohibited articles into the strong magnetic field area.

5.2 Maintenance of front release system

Prevent it from being placed before impact, try not to move it, and be careful not to move the connector of the cable during cleaning.

5.3 Control Cabinet Maintenance

(1) Ensure the normal operation of UPS.

(2) If UPS is used for power supply and power failure is required for a long time, please stop the experiment in time. UPS can be used for the spectrometer to run for about 1 hour when the experiment is not done. If power failure is long, please shut down or take other measures.

(3) The control cabinet shall use vacuum cleaner to remove sundries and dust at least every month.

(4) Clean the fan dust net in the cabinet:

(5) For the main control system and magnetic control system, the fan is located at the bottom of the chassis. Screw a fixing screw by hand from the front of the chassis, pull out the fan disc, clean the fan with a wet towel, pay attention to the towel not dripping water, and prevent cable joints and fan motors from being damaged. After cleaning, wait for the water to dry before inserting the fan into the chassis.

(6) For the power amplifier, you need to remove the front panel of the power amplifier and clean the dust net inside.

5.4 Laboratory Maintenance

(1) It is forbidden to bring ferromagnetic articles into the laboratory. Those that must be brought in shall be strictly managed and shall not enter the magnetic field warning area.

(2) Ensure the cleanliness of the workplace, orderly placement of desks, chairs, articles, etc., and no surplus items shall be piled up.

(3) Laboratory personnel should wear special experimental clothes and replace special slippers when entering the laboratory.

(4) Special management shall be carried out for samples with low boiling point, toxic, flammable and explosive.

5.5 Cleaning

(1) Lab cleaning shall be carried out regularly, and brooms and mops shall not contain ferromagnetic articles.

(2) During the experiment, personnel should not enter the 5 Gauss line.

(3) Use the vacuum cleaner to suck out sundries regularly. Do not enter the 5 Gauss line for the main part of the vacuum cleaner.

(4) The surface of the magnet can be cleaned with dry soft cloth, which can be slightly soaked with water or stained with a small amount of alcohol.

(5) Use a vacuum cleaner to suck out sundries in the control cabinet. The surface of the cabinet can be wiped with soft cloth, which can be slightly soaked with water or stained with a small amount of alcohol.

CAUTION *Do not use acetone to clean the surface of any parts of the spectrometer. Acetone will damage the paint and plastic parts on the surface of the parts.*

6 Faults and Treatment Methods

6.1 Fault Identification

Q.One apologizes for the failure of NMR spectrometer, which will affect your normal use and may cause certain direct or indirect economic losses. When there is a fault, Q.One is committed to handling the fault as quickly as possible to minimize your losses, but it is especially important for you to provide Q.One with accurate fault information and help.

This section lists some common problems of Quantum-I Plus NMR spectrometer for spectrometer management personnel to preliminarily judge the failure points of spectrometer,

so as to facilitate Q.One engineers to carry out on-site treatment, and also for spectrometer maintenance personnel to carry out preliminary treatment with reference to the solutions to corresponding problems.

Both the Quantum-I *Plus* NMR spectrometer control system and SpinStudio have set up necessary error marks or messages for users to identify possible faults of the spectrometer.

In the Quantum-I *Plus* NMR spectrometer control system (hardware), the user can determine the spectrometer status through the display status of LED or LCD. Please read the contents in Section 3.2 to judge whether the display is normal. In most cases, when the red LED is always on or the green LED is not on, an error occurs. Through the contents of Section 3.2, you can initially determine that there is a problem with a certain part of the system.

SpinStudioJ will give some error messages, and you can identify whether there is a problem with the spectrometer through the error status.

6.2 Repair Report

When the Quantum-I *Plus* NMR spectrometer fails, please report for repair in time. You can choose the following repair methods:

1) Call the company's customer service number. Please see product consultation, sales, technical support and repair for contact information.
2) Report for repair through Q.One WeChat public number.

When applying for repair, please provide Q.One with detailed fault description, such as error information given by SpinStudioJ, hardware indicator light, etc. If necessary, please provide photos or spectrum to facilitate Q.One to judge the fault point and speed up the fault processing.

Q.One engineers may need your help in determining the failure point. Please support Q.One's work. We would like to express our gratitude.

6.3 Troubleshooting

When the Quantum-I Plus NMR spectrometer fails, especially when the spectrometer is

under warranty, Q.One does not recommend that you handle the failure of the spectrometer yourself. Some simple problems can be handled by users themselves, such as replacing fuses, but it is best to do so under the guidance of Q.One engineers.

The spectrometer administrator should not open the chassis or repair or change the internal structure of the system when dealing with the spectrometer failure. During the warranty period, this behavior will lead to the suspension of the service promise provided by Q.One. If spectrometer maintenance personnel determine that it is necessary to open the chassis or change the equipment, please carefully read the contents in the safety summary, warnings, precautions and other sections of this manual, and pay attention to the safety warning signs on the chassis to ensure that no direct or potential personal injury will be caused. When you cannot solve the problem, please contact Q.One in time.

6.4 Common Trouble Handling Methods

(1) The forward LCD does not display the correct channel status

Please check whether the cable on the front and rear interface J7002 is completely loose.

Please check whether the cable connection of J2002 is loose on the cabinet side.

The above steps cannot eliminate the problem, please contact Q.One.

(2) The power supply of each subsystem of the control cabinet cannot be turned on.

Please check whether the PDU has displayed the voltage value and whether the voltage is correct.

Check whether the three-in-one switch is on, and if so, check whether the fuse in the three-in-one switch is in good condition.

When replacing the fuse, turn off the power supply of the corresponding position of PDU, remove the power plug and replace the fuse at the power socket. Q.One has attached a spare 4A delay fuse with a length of 5 × 20 mm when the spectrometer system is shipped. You can use it directly.

(3) The indicator light is incorrect when the main control system is started.

The main control system should enter the normal operation state after turning on the power switch for about 1 minute. You can check the status of the indicator light on the front panel of the main control system according to Section 3.2. 1. If there is any abnormal phenomenon, you can turn off the power supply of the main control system, turn it on again after 1 minute, and then check again.

If you are still in the error state, please contact Q.One in time.

In general, if the main control system does not start normally, SpinStudioJ will not be able to connect to the console and will display a connection error.

(4) Sample cannot eject

In order to ensure the safety of the spectrometer, the air control system is equipped with air pressure and humidity monitoring functions. When the air pressure is insufficient or the humidity is too high, the air control system will stop working.

Please check whether SpinStudioJ has any errors in displaying air pressure or humidity.

Check whether the cable plug from air control panel J6901 to magnetic control panel J6802 is loose.

If the problem still cannot be solved, please contact Q.One in time.

(5) There is no gradient effect in the spectrum.

Please check whether the position of the enable switch of the gradient power amplifier is enabled.

Please check whether there are non-green lights on the front panel of the gradient power amplifier. If so, please dial the enable switch to reset the gradient power amplifier.

Please check whether the cable plug between the gradient power amplifier and the probe is loose.

If the problem cannot be resolved, please contact Q.One.

(6) SpinStudioJ Reports Connection Errors

Please first confirm that the startup status of the main control system is correct according to the startup status of 3.2. 1, otherwise please follow the treatment method of Question 3.

If the start-up state of the main control system is normal, please check whether the network cable between each circuit board of the main control system and the router is loose. Generally, you can also use ping command for connection detection.

Please check whether the network cable connection between the cabinet and the workstation is normal.

Please check that the workstation network card is working normally.

If the network connection is normal, please contact Q.One.

(7) More questions

Please pay attention to the Q.One website. Problems that Quantum-I Plus NMR may encounter during use can be accessed on the Q.One website and will be updated continuously.

In the process of using Quantum-I Plus NMR spectrometer, if you have any problems, please contact Q.One in time. Q.One will provide detailed treatment opinions or directly send service personnel to the site for treatment.