University of Colorado 800 MHz NMR Facility:
Facility Overview

Each user of the 800 MHz NMR spectrometer is required to undergo a brief orientation and get checked out on the instrument by the facility manager. This document will serve as a brief overview of the facility, spectrometer hardware, and some very basic procedures. Additional documents will contain more specific instructions and information. In addition to this document, "Setting Up Experiments" lays out a number of policies that must be followed every time you get on the instrument and is required reading. These and other documents will be available in hardcopy or may be downloaded in PDF format from the laboratory webserver, located at http://cunmr800.colorado.edu.

Location and Access

The 800 MHz NMR spectrometer is in the northwest corner of the "Center for Innovation and Creativity" (CINC, room 193A), located at 1777 Exposition Drive, on the corner of Exposition and Fisher Drives across from the RTD bus garage.

Access to the 800 lab is by keycard only. Using your BuffOne card or a guest card, you can enter the building at any time through either the front door or the exterior door in the northwest corner of the CINC building. Access to the lab itself is through another card reader on the small door next to the large double doors facing the loading dock. The facility manager has access to the keycard system and can grant or revoke access privileges at any time.

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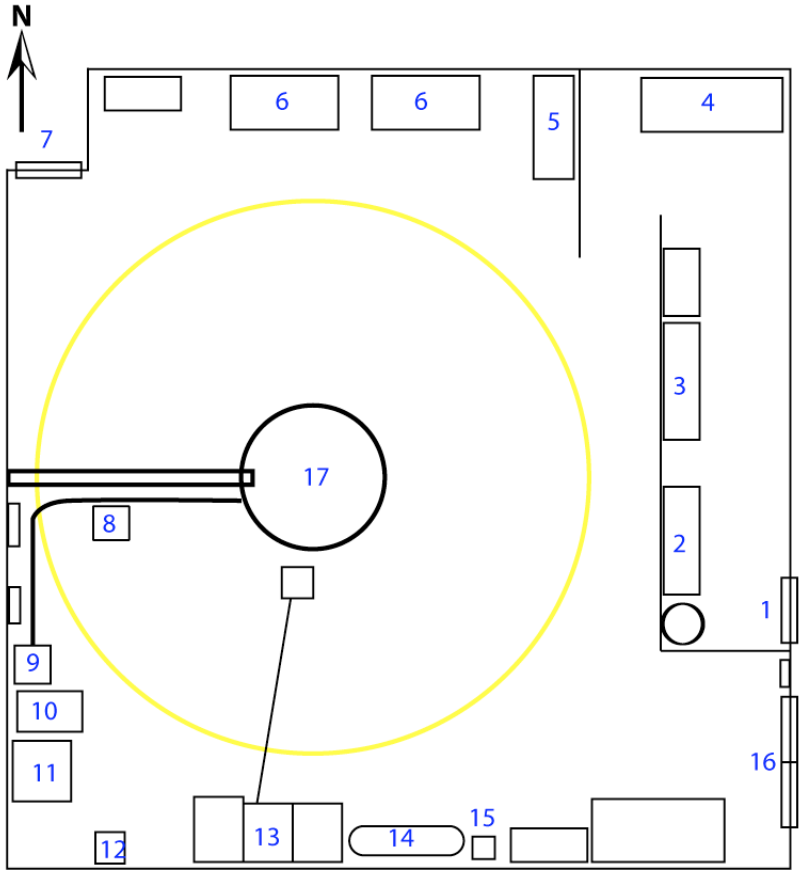
Layout of the Laboratory

The following image shows the basic layout of the NMR laboratory. General access from the outside is via the northwest door (above the north door, #7), followed by the smaller east door (#1) using your BuffOne or guest card.



1 door - keycard access
2 air drying equipment
3 storage - tools and files
4 food and coffee area
5 firewall and webserver
6 workspace / desks
7 north door
8 FTS (VT chiller)
9 vacuum pumps
10 magnet monitor
11 chiller for cold probe
12 UPS for console
13 console
14 Sun workstation
15 sample refrigerator
16 doors for large equipment
17 800 MHz magnet

Safety Information and Emergency Procedures

For the most part, the hazards present in the 800 facility are the same as those in any other NMR laboratory: strong magnetic fields, high voltage, and cryogens. Do NOT bring any tools or other metal items inside the 5 gauss line (the large yellow circle painted on the floor) unless you are either 100% sure that they are non-magnetic or you have the approval of the facility manager. Even more importantly, do not get between the magnet and any large metallic objects - if you get stuck in between you could suffer broken bones, suffocation, and even death. We do have a method to quench the magnet if this should happen, but only as an absolute last resort.

Another major hazard is cryogens, which can cause severe frostbite. Gloves and safety glasses should be worn when working with liquid nitrogen and helium. Additionally, in the extremely unlikely event of a quench, you should get down near the floor and exit the room immediately. Wait until the helium gas has dissipated before re-entering the space.

If an emergency should occur, immediately call the facility manager. The one caveat to this is that if some requires immediate medical attention, get help for him or her before attempting to contact anyone else. Emergency phone numbers are posted on the white board near the console, at the end of this document, and on the outside of all doors into the NMR lab.

Spectrometer Overview

The 800 MHz spectrometer is in many ways similar to the other Varian Inova systems you may be used to, but there are several differences. Our 800 MHz instrument is a 4 channel instrument with waveform generators on all four channels. A triple axis gradient amplifier is available, and our current probe is a Varian HCN probe with triple axis gradients. A cold probe is expected at some point in the future.

The console itself consists of three cabinets. The leftmost cabinet contains the frequency synthesizers (PTS), the digital cardcage, the VT control and heater unit, and the RT shim supply. The center cabinet contains the RF cardcage, gradient amplifier, proton amplifier, and the main power supply. Finally, the taller cabinet on the right holds the other amplifiers and controls for adjusting the spinner. The low band amplifiers are quite powerful (1 kW) and are capable of damaging the probe and/or your sample if too much power is used.

Scheduling Time on the 800

Time on the instrument will ideally be shared equally among the three institutions. Time will be charged as actual costs based on a percentage of time used, with instrument down time shared by all three institutions.

Currently, you can request time by sending email to the facility manager detailing what experiments you intend to run and how much time you expect to need, and you will be placed in the queue as time is available. Make sure you include any special details that might affect scheduling (*i.e.* grant deadlines, unstable samples). Finally, make sure to include pulse code and parameters for any non-standard experiments to be approved in advance of your time (a separate document on moving pulse sequences to the 800 will be available). A more formal schedule will eventually be put into place.

Appropriate arrangements should be made far enough in advance if you need to travel to Boulder, have samples shipped and/or changed, or otherwise require direct assistance with setting up your experiment. If for any reason you can not use your scheduled time, you should inform the facility manager as soon as possible so that someone else can get on the instrument.

Computer Policies

Each laboratory will have one account on the Sun workstation controlling the spectrometer. Access to this computer from outside is strictly controlled by a firewall, so you must make arrangements in advance for remote access to your data (a separate document will be available for accessing data and running the spectrometer remotely). At the moment, we have no quotas, but it is your responsibility to move large data sets off the system in a timely manner. Backups

will be made to another computer and to permanent media on a regular basis; however, you are ultimately responsible for your own data.

The entire lab is set up for both wireless and wired internet connections if you choose to bring your own laptop. We additionally have two public access computers: a PC laptop that is also used to control keycard access to the lab, and a Linux desktop that runs the lab webserver. The latter has NMRPipe software installed if you need to check your data, although it is relatively slow.

Contact Information

What follows is the address of the NMR facility, shipping information for sending samples, and contact information.

800 MHz NMR Laboratory
1777 Exposition Drive, Room 193A
Boulder, CO 80301

- if shipping packages directly to the 800 facility via UPS or FedEx, specify delivery to the loading dock and make arrangements for someone to meet the shipment in advance - there is no receiving department in our building

303-492-1100 (lab phone)

- For routine packages and samples, the Chemistry department stockroom is always staffed:

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