

NMR CENTER RULES

1. Use of the NMR Center

Only authorized users may enter the NMR Center. Unauthorized persons should never be present in the NMR Center, except to receive training.

2. Use of the Spectrometers

Users must receive appropriate training before using the spectrometers. This requirement involves arranging for and attending as many training sessions as are necessary with a qualified NMR user in your research group, and then demonstrating proficiency on the spectrometers to one of the NMR Staff. Qualified users will be given a signed key request form from the director. Other training arrangements may from time to time be required at the discretion of the laboratory director.

3. Access to the Spectrometers

Time on the spectrometers must be reserved either by logbook or on-line at <http://xray.bc.edu/nmr/admin.php> Each research group has been issued a username and password for the on-line reservation system. Users may access the reservation system from any authorized computer on the BC Network. In the event that reserved time on a spectrometer cannot be used, it is the user's responsibility to cancel the reservation on-line as soon as possible so that the time may be used by others operators. The time displayed on BC telephones and computers shall be considered the "official" time source for NMR scheduling and reservations. That time will be reproduced as faithfully as possible on the wall clock in the NMR Center. Accounting software is installed and running on all spectrometers. Login times are being recorded and compared with reservation requests. Rules for accessing the spectrometers are the following:

1. The **VNMR 400 spectrometer (nmr14, department 400)** is now running in open access mode 24 hours a day, 7 days a week. Users can reserve 20 minute time slots from 8 am to 8 pm by log book sign-up and from 8 pm to 8 am for up to 12 hours by on-line reservation.

2. The **MR-400 spectrometer (nmr13)** will continue to be used by the Hoveyda group exclusively (Hoveyda group users are not limited to this machine) and may be used for 20 minute blocks of time from 8 am to 8 pm 7 days a week by log book sign-up and for up to 12 hours from 8 pm to 8 am overnight by on-line reservation.

3. The **500 INOVA spectrometer (nmr11, old 500)** may be used 7 days a week between 8:00 am and 8:00 pm by log book sign-up for a maximum of 20 minutes, and between 8:00 pm and 8:00 am by on-line reservation for up to 12 hours.

4. The *VNMRS 500 spectrometer (nmr18, new500)* will be available to all users 7 days a week by log book sign-up between 8:00 am and 10:00 pm for a maximum of 20 minutes, and between 10:00 pm and 8:00 am by electronic sign-up for up to 10 hours.

5. The *VNMRS 600 spectrometer (nmr19)* is available 7 days a week from 8 am to 8 pm for 20 minute periods by log book sign-up, and from 8 pm to 8 am by on-line reservation for up to 12 hours.

Exceptions to these rules may be granted occasionally. When they are, all users will be notified by email and the exception will be posted by the spectrometer.

4. Behavior in the NMR Lab

Users of the NMR Center must behave in a manner that is safe for themselves and others in the lab, and minimizes the potential for damage to the instruments. They also must behave in a way that supports the most efficient and accurate collection of data. Both of these objectives necessitate behavior that does not distract the user or others in the lab from their work on the spectrometer. Socializing in the NMR lab or carrying on conversations unrelated to the sample being analyzed, for example, are never appropriate behaviors. In addition to conforming with safety measures specific to the NMR lab, all behavior in the NMR Center must conform to the regulations prescribed in the NMR Center, Chemistry Department, and University Safety Documents. Eating and drinking in the NMR Center is prohibited, for example.

5. Standard Practices on the Spectrometer

When the spectrometers are used, the users are responsible for the quality of their data. This means that appropriate parameters and careful shimming are essential to every experiment. Shim sets that meet instrument specifications are saved regularly by the directors and may be recalled simply by any user. Users may also save their own “good” shims and recall them simply. Also, careful pulse width and power level calibrations are made regularly and saved in the standard parameter files. Users can also save their own parameters sets. Therefore, the quality of user’s data is not dependent on the skills or sample characteristics of the person preceding them on the spectrometer. Users should begin each session on the spectrometer by calling in a standard (or user defined) set of parameters and shims. Trained NMR users all have been instructed in these procedures, but a set of instructions will be provided to any user that requires them.

6. Special Operations on the Spectrometers

Procedures such as changing probes or performing variable temperature NMR require additional training from the director of the Center. Only users with permission to perform these operations may do so. In order to minimize the potential for damage to

the instruments, the director of the Center will attempt to minimize the number of probe changes on the spectrometers. Also, some special operations (e.g. low temperature NMR) require cryogen storage devices not normally kept in the NMR lab. Therefore, users must arrange special experiments or probe changes ahead of time with the director of the Center. In addition, if help is required to perform a particular experiment, that time must be arranged for in advance so that users can receive the full attention of the director.

7. Problems with the Spectrometers

If a user discovers or causes a problem with the spectrometer (broken sample, computer malfunction, printing problem, etc.) they have two responsibilities: first to prevent further damage to the system or its operators, and second to notify the director of the problem. Further damage to the spectrometer is best prevented by warning other users not to use the instrument. This can be accomplished with a note placed over the keyboard or in some other conspicuous location on the spectrometer. Reporting the problem to the director should be done by telephone, in person, or by email. The user must indicate the material in the sample, the solvent used, and any information about its toxicity if a sample is broken. Vendors will not repair probes without this information.

Problems with access to the NMR instruments or other user related problems should be reported to the directors of the NMR center either in person, by email, or through their faculty advisor. The importance of reporting difficulties in a civil and respectful manor cannot be overstated. Disrespectful, angry, or aggressive behavior directed toward the users of the facility or the facility staff will not be tolerated and will result in the loss of NMR privileges.

Please note that no user should attempt to fix or adjust a system that has malfunctioned. Air pressure adjustments, rebooting of computers, restarting spectrometers, etc. should all be performed by one of the directors, a manufacturer's representative, or someone else in the Chemistry Department who has received training. Attempts to perform corrective measures by untrained users almost always result in more damage to the system than the original problem.