

NMR Center News

**It's time to
backup
your NMR
data!!!!**

December 5, 1997

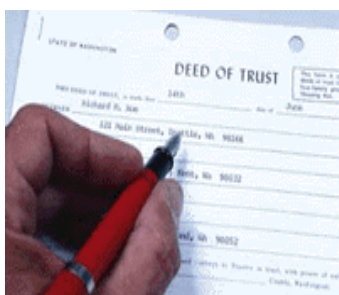
Volume 1, Issue 4

Many NMR books and articles refer to 'Zeeman splitting' of nuclear magnetic energy levels. In fact, Zeeman had nothing to do with NMR; his relevant papers were published in 1897.

In a paper published in the Philosophical Magazine, P. Zeeman reported on the "Influence of Magnetism on the Nature of the Light Emitted by a Substance". He found that the well known yellow D lines emitted by sodium vapor

NMR Instruments Tune up Schedule During the Holidays

Our NMR instruments have been overworked for several months without major breakdown. Now is a good time for us to clean up disks, retune the probes, shim the magnets, wash the filters



The tune-up schedule for each instrument is as

follows:

QE300:

12/8/97

INOVA400:

12/10/97

GN500:

12/9/97

Omega600:

12/11/97

UNITY400:

12/12/97

Please back up your own data by **December 20, 1997**.

If you don't know how, please make an appointment with us. We will help you to back up your files on a tape, zip disks, floppy disks or a writable CD ROM.

Back up Your DATA on INOVA400

If you have saved NMR data on INOVA400, you can back up your data as following:

1. Get a DC6150 Data cartridge tape from the stockroom.
2. Insert the tape into the tape drive. See the instructions on the tape drive.

3. Open a VNMR window by double clicking the vnmr icon.

4. Find your data directory and type: **tar cvf /dev/rst4 your_file_names.**

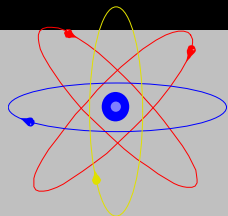
5. After backing up your files, you may delete the files on the disk. Type: **rm -r file_names.**

Spin Diffusion in NOE Measurement.

Spin diffusion is a T1 phenomenon frequently observed in NMR of macromolecules. In the limit of $w\tau_c \gg 1$, the rate of transfer of spin energy between nuclei becomes much larger than the rate of transfer of energy to the lattice. This results in longitudinal relaxation rates of protons within the molecule which all tend to the same value. Since the NOE is dependent upon T1, in the presence of spin diffusion, this parameter will no longer be specific for proximal spins. In the extreme case, a homogeneous negative NOE will be observed throughout the whole spectrum. In practice, spin diffusion is evident in the generation of relayed NOEs in either 1D NOE difference or 2D NOESY spectroscopy. Under these conditions there is no simple relationship between the magnitude of the NOE and the internuclear distance, and for this reason NOESY spectra should only

How many NMR users are able to operate all NMR instruments in the NMR Center

All NMR instruments	6
GN500, INOVA400, QE300	12
INOVA400, QE300	40
QE300	86



were broadened when the sodium chloride sample was heated and placed in a magnetic field. Later work showed that the broadening was actually a splitting of the lines, and the term 'Zeeman effect' was applied to this phenomenon in optical spectroscopy. The term was generalized to include the splitting of energy levels through interaction with a magnetic field. Thus, the Zeeman interaction is the dominant term in

TIPS for INOVA400 Users

On the INOVA400, there are several operations that can be used to make spectrum acquisition easier. For example, your data can be saved automatically when data acquisition is completed, or the system will automatically display the current spectrum with an increased signal over noise ratio when the next block size of scans is finished. Your spectrum can even be plotted out automatically. The following description will show you the detailed

procedures:

Checking the up-to-date signal over noise ratio:

After the standard parameters are loaded, for dilute proton experiments, set **bs=16**, **nt=256** or more. For carbon experiments, set **bs=32**, **nt=1024** or more. Type **wbs='wft'**. Enter the command **au** instead of **ga**. You can measure the signal-to-noise ratio after 16 scans. When the signal over noise ratio is high enough, enter command **aa** or click Abort acquisition button.

Saving the data automatically after data acquisition is completed:

Load the standard experiment parameters and adjust acquisition parameters as needed.

Change to a specific sub-directory in which you want to save your data.

Type **wexp='svf(\filename\')**. Beware of the single quotes and backslashes. Enter the command **au** instead of **ga**. After the experiment is complete, the data will be automatically saved on the hard

HOW to Take a 2D COSY Spectrum on INOVA400

disk.

1. Load the standard proton parameters and take a proton spectrum as a reference.
2. Use two cursors to set the spectral width(use command "movesw").
3. Type cosy for loading the cosy parameters.
4. If you have a 30 minute time slot, setup the experiment as follows:
a. nt=4, np=1024, ni=256

wexp='svf(\filename\')' ,
gain=35

- c. Type time to check total experiment time and then type au to start acquisition.
- d. You may have to transfer the data to the data station to process and plot data.
5. If you have one hour or more time, you can setup the experiment as follows:
a. nt=16, np=2048, ni=512
You will have much better

spectral resolution.

6. COSY data processing:

a. load the data and type **wft2d** for magnitude COSY and **wft2da** for phase sensitive COSY. Use **vs** to adjust peak intensity. The following commands are very useful:

foldt
plcosy(12,1.2)
pcon(12,1.2) page

Some Important UNIX Commands

Tape Operation:

On SUN (INOVA400, Omega600)
tar cvf /dev/rst0 file_names

Retrieve data from above format into INDIGO
tar xvf /dev/tapens

FTP Operation

ftp 170.140.39.175
login and passwd
ftp>binary — set to l
ftp>get file_name
ftp>bye — quit
ftp>cd — change DIR

ftp>ls — list files
ftp>cdd — change local dir

File Operation:

mv file_1 file_2
mv -if dir1 dir2
cp file_1 file_2;
cp -r dir1 dir2
rm file_name
rm -r directory
more file_name

vi editor:

vi filename
:set showmode
:set nu

:num goto line num

:set flash

:w file_name

w: /dir/filename

ctr -H erase a char

ctr -u kill the line

ctr -w erase a word

ctr -R redraw the screen

dd delete current line