

Current Developments

The Camille and Henry Dreyfus Foundation, Inc. has awarded the chemistry department a \$30,000 matching grant (SG-03-067) toward the purchase of accessories to upgrade the Bruker DPX Avance-300. The purpose of the grant was to allow the use of the NMR by larger classes.

The number of students doing hands-on experimentation with FTNMR can be increased six- to eight-fold by collecting data through the night and weekends, as well as during laboratory hours, and by processing data off line instead of at the spectrometer console, and by using a pulse field gradient probe. The speedup will not only give all first year chemistry students direct access to the spectrometer, but it will enhance advanced courses by allowing students repeated use of the instrument, with a wider choice of applications. In advanced organic chemistry, this is especially valuable in 2-D NMR, which is time-consuming.

The justifications for the equipment requested from Dreyfus are as follows:

- i. **Pulsed gradient probe:** This was needed to reduce time needed for data collection. Data collection rate is limited many times by slow relaxation times following each pulse. The upgraded probe will drastically reduce the recycle time for an experiment by forcing the nuclear spins to attain equilibrium more rapidly.
- ii. **Electronics upgrade:** This is needed to accommodate the pulsed gradient probe to the present instrument.
- iii. **The computer software and PC license upgrades:** The WINNMR upgrade was deemed necessary to enable students to process data off-line, that is, independent of the spectrometer. With computer network access, some students can do data analysis while others use the spectrometer. A PC network license from Bruker is required to interface the NMR spectrometer to the campus-wide computer network, enabling the student to access files on PC's.
- iv. **Sample autoloader:** An automatic sample loader enables unattended data collection at all hours. This is the most critical acquisition for increasing student use of NMR, particularly in larger classes.

Specifically, the he following accessories will be obtained from Bruker in the near future:

Automatic Sample Changer - B-ACS-60

WI NMMR software Upgrade for Windows

GRASP gradient spectroscopy upgrade

I nverse Broadband PFG probe