D.M. Grant NMR Center Instrumentation

<u>General</u>

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Services, Equipment and Users

Main Services

The D.M. Grant NMR Center provides the University of Utah research community access to high-resolution solution NMR spectrometers. Basic NMR training and consultation are available.

Major Equipment: Liquids NMR

NMR Center liquids instruments were all manufactured by Varian/Agilent and include one 500 MHz (¹H) four-channel (¹H, ²H, ¹³C, ¹⁵N) spectrometer named 500a, one 500 MHz (¹H) threechannel (¹H, X-low-band, X-low-band, wherein X-low-band refers to all nuclei up to a resonance frequency of about 200 MHz, e.g., ³¹P) spectrometer named 500b, and an 800 MHz (¹H) fourchannel spectrometer named dd800. All instrument RF-consoles feature entirely digital receiver sections that eliminate virtually all of the inherent quadrature detection artifacts present in analog designs. The 500a instrument was installed in May, 2012, and features a high-sensitivity cold-probe detection system that provide an increase of approximately 4x over the conventional room-temperature probe design. The 500a instrument is designed with application to biological macromolecules as its primary target, but is extremely useful in any applications requiring highsensitivity detection of ¹H and/or ¹³C resonances (e.g., low sample concentration). The 500b instrument was installed in October of 2011, and is equipped with a number of direct X-nucleus detection and indirect ¹H-detection probes. The 500b instrument is an excellent general utility instrument that is capably of VT operation over the range from about -100°C to about +80°C. The dd800 instrument was installed in the summer of 2010 and is equipped with two probes, an indirect ¹H, ²H, ¹³C, ¹⁵N probe that is most useful for study of biological macromolecules, and a direct X-low-band probe (¹H-decouple) that is most useful for application in synthetic chemistry and materials science.

Major Equipment: Solid State NMR

The NMR Center is also home to two older ChemMagnetics NMR solid-state instruments operating at 200 MHz (¹H) and 400 MHz (¹H). These instruments were installed in the late 1980's but remain completely operational. Both systems support standard CP/MAS experiments with high power ¹H and X-low-band operation. The instruments were designed to carry out magic-angle turning experiments that provide high-precision measurements of chemical shift tensors (e.g. slow-turning FIREMAT experiments), which can provide unique structural information. The 200 MHz instrument is equipped with probes that support 5 mm and 7.5 mm rotors with turning speeds of approximately 12 kHz and 7.5 kHz respectively. The 400 MHz instrument is equipped with a 7.5 mm probe that supports maximal turning speed of

approximately 7.5 kHz. The emphasis of these instruments has been and remains magic-angle slow turning experiments in which rotational frequencies are typically less than 2 kHz. In February of 2009 a new digital console was added to the laboratory that provides access to the standard range of multidimensional/multinuclear CP/MAS experiments for the instrument operating at 200 MHz (¹H).

FIREMAT reference: Alderman, D. W.; McGeorge, G.; Hu, J. Z.; Pugmire, R. J.; Grant, D. M. Mol. Phys. 1998, 95, 1113