SPECTROMETER CAPABILITIES AND SPECIFICATIONS

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I. Overview of Spectrometer Specifications

The JB Stothers NMR Facility in the Department of Chemistry at Western houses three liquids NMR spectrometers: the Varian Inova 400, the Varian Inova 600, and the Bruker Avance III HD 400. A summary of the general features of the three current liquids NMR spectrometers is presented in Table 1.1. An explanation of the terms can be found in the last section of this document.

Table 1.1. General Specifications of the Bruker 400, Inova 400, and Inova 600

Spectrometer Name	Console Information			NMR Magnet	Probe Tuning	Autosampler	Software
	Manufacturer	Model	Install Year				
Bruker 400	Bruker	Avance III HD	2017	Oxford AS400/54	Auto	24 samples	TopSpin3.5 / Icon5
Inova 400	Varian	Inova	2000	Oxford AS400/54	Manual	No	VnmrJ 4.2 MI
Inova 600	Varian	Inova	2000	Oxford AS600/51	Manual	No	VnmrJ 4.2 MI

II. Probe-dependent Specifications

In Table 2.1, specifications that are dependent on the NMR probe in use are presented. Although most of the spectrometers have several probes available for use, generally the same probe is used at all times.

Table 2.1. Probe Specific Specifications of the Bruker 400, Inova 400, and Inova 600

Spectrometer	Usual Probe	Tuning	Capabilities with Usual Probe								
			^{1}H	^{1}H{^{19}F}	^{13}C	^{19}F	^{19}F{^{1}H}	^{31}P	X{^{19}F}	Other Nuclei	Variable Temperature
Bruker 400	5mm SmartProbe	Auto	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes	No
Inova 400	5mm Direct Detection Autoswitchable HFCP	Manual	Yes	No	Yes	Yes	No	Yes	Yes	Yes[a]	-80 to +130 °C[b]
Inova 600	5mm Direct Detection AutoX-DB	Manual	Yes	No	Yes	Yes[a]	No	Yes[b]	Yes	Yes[a]	-30 to +130 °C

[a]Requires manual tuning of the probe
[b]Requires the use of liquid nitrogen for cooling

III. Spectrometer Sensitivity

The sensitivity of an NMR spectrometer is determined by acquiring an NMR spectrum of a standard sample and determining the ratio of the intensity of the signal to a set region of noise (i.e. the signal-to-noise, S/N). The sensitivity of the three current liquids NMR spectrometers, and the old Mercury 400, is presented in Table 3.1.

Table 3.1. Sensitivity Comparison of the Bruker 400, Inova 400, and Inova 600

Spectrometer	^{1}H S/N[a]	^{13}C S/N[b]	^{19}F S/N[c]	^{31}P S/N[d]
Bruker 400	480:1	210:1	310:1	250:1
Inova 400	190:1	130:1	160:1	100:1
Inova 600	410:1	320:1	390:1	195:1

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IV. Description and Glossary

Liquids NMR spectrometers and probes are classified based on several criteria. A brief description of each criteria is provided below.

The Spectrometer Company and Model
Currently, the leading manufacturer of NMR spectrometers in North America is Bruker Biospin, a company based out of Germany. Before folding its NMR operations in 2010, Varian, Inc, a company based out of California, was Bruker's main NMR competitor. Each company has different models of spectrometers depending on the desired specifications; models constantly change over the years as NMR technology improves. We have both Bruker and Varian NMR spectrometers in the JB Stothers NMR Facility.

The Magnetic Field Strength
The resonance frequency of a particular nucleus is directly proportional to the magnetic field strength. As a result, the magnetic field strengths for NMR spectrometers are usually described by the ^{1}H frequency at that particular magnetic field strength, rather than in Tesla (T). For example, on a Varian Inova 600 spectrometer, the ^{1}H frequency is about 600 MHz, corresponding to a magnetic field strength of 14.1 Tesla. On a Varian Inova 400 spectrometer, the ^{1}H frequency is about 400 MHz, corresponding to a magnetic field strength of 9.4 Tesla. In general, the greater the magnetic field strength, the greater the sensitivity and resolution of the instrument.

Variable-Temperature Capabilities
In order to perform experiments above or below room-temperature, a variable-temperature controller and heat-exchanger (for low-temperature experiments) is required.

Odd-Nuclei Capabilities
The majority of NMR spectrometers can perform ^{1}H and ^{13}C NMR experiments. Depending on the NMR probe, number of channels, and type of amplifiers, experiments on other nuclei can be performed as well.

Tuning
The NMR probe is setup (or tuned) to observe certain nuclear isotopes. Typically, by default, one of the probe's channels is tuned to ^{1}H, while the other is tuned to ^{13}C. If the probe is not properly tuned to your nuclear isotope of interest, you will not be able to observe any signal. To observe any non standard nucleus, the probe must be either tuned by the user or using the spectrometer's automatic tuning module.

Spectrometer Sensitivity
The sensitivity of the spectrometer is described by the signal-to-noise (S/N) ratio for a specific nuclear isotope. The S/N ratio is the ratio of the intensity of a specific peak in the NMR spectrum of a standard sample versus the average intensity of a set region of noise. The spectrum used to determine S/N is acquired using one scan with a standard set of parameters (i.e. specific spectral width, relaxation delay, etc.). Some common sensitivity test samples are listed in the table below.

Table 4.1. Standard Samples used for Sensitivity Testing

Nucleus	Sample	Solvent	Concentration
^{1}H	Ethylbenzene	$CDCl_3$	0.1% v/v
^{13}C	*p*-Dioxane	C_6D_6	40% v/v
^{15}N	Formamide	DMSO-d_6	90% v/v
^{19}F	Trifluorotoluene	$CDCl_3$	0.05% v/v
^{31}P	Triphenyl phosphate	Acetone-d_6	0.0485M

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NMR Probe

The NMR probe resides in the NMR magnet and the NMR sample sits inside the probe's radiofrequency coil. During an NMR experiment, the probe receives the radio-frequency pulse from the spectrometer, transmits the pulse to the sample, receives the NMR signal from the sample and directs the signal back to the spectrometer. There are many types of probes available, and the probes differ by the following:

Indirect vs. Direct Detection: A liquids NMR probe typically contains two coils, one for high-frequency ^{1}H and/or ^{19}F pulses, and another for lower-frequency pulses (eg. ^{13}C, ^{31}P). An indirect-detection probe has the high-frequency coil nearer the sample than the lower-frequency coil and as a result the probe provides superior results for ^{1}H 1D or ^{1}H detect 2D NMR experiments such as a HSQC. A direct-detection probe is reversed, such that the lower-frequency coil is nearer the sample and the probe provides superior results for 1D NMR experiments on nuclei other than ^{1}H or ^{19}F. A new generation of probes combines the best features of both an indirect and direct-detection probes.

Number of channels: NMR probes have different number of channels, which determine the number of simultaneous pulses that can be applied to the sample at a given time. For example, a 2-channel probe can receive pulses at 2 unique frequencies, usually at the ^{1}H and ^{13}C frequencies. Some probes contain as many as 5 unique channels, but 2 to 3-channel probes are the most common.

Tuning range of channels: Each channel will have a specific tuning range. The tuning range may be limited to that of a single nucleus or the range may encompass a broad range of nuclei. Each channel is labeled by its tuning range. For example, an "H" channel can only tune to ^{1}H frequency, a "P" channel can only tune to the ^{31}P frequency, an "X" or "Y" channel can tune to a broad range, generally between ^{31}P and ^{15}N. Thus, an HPX probe is a 3-channel probe with dedicated ^{1}H and ^{31}P channels, plus a third channel that can tune to a broad range of frequencies.

Coil diameter: The standard rf-coil is designed to accept a 5.0 mm outer diameter (o.d.) NMR tube. Other probes are designed to be used with 3.0 mm o.d. NMR tubes or 10.0 mm o.d. NMR tubes.

VT capable: Only specifically designed probes are designed for variable-temperature NMR experiments. The temperature range is generally probe-specific.