NMR Sample Tube Guidelines

The great variety of sample tubes available for NMR can be very confusing. On one hand, the manufacturer wants to sell you the most expensive tube that they can, while on the other hand, the researcher wants a tube that will give a good spectrum at minimum cost. The following is a rough guide to the types of tubes available.

# MHz Rating

The “MHz Rating” that many manufacturers put on their tubes is nothing but marketing hype. While it is true that a higher field instrument will benefit from a more precise tube, a tube rated at “200 MHz” will work just fine in a 500 MHz or 600 MHz instrument for many routine samples. For many samples, the decrease in resolution resulting from using a lower grade tube will not be noticeable.

# Economy tubes made from N51A glass (< $5 each)

These are the lowest priced tubes. Examples would include Wilmad “Economy” series tubes, Norell XR55 tubes, Norell “Standard” tubes, Aldrich “Thrift” tubes and others. There are a number of issues with these tubes:

* N51A glass can contain up to 1200 ppm iron, which can cause problems with resolution and shimming, especially at higher fields.
* The manufacturing tolerances of these tubes are much lower than for precision tubes. The spectrometer manufacturer specifies 4.95 +/- 0.02 mm for sample tubes, while I have seen these tubes vary from 4.89 to 4.98 mm. They also tend to be “out or round” and can vary in diameter along the length of the tube.
* The thermal coefficient of expansion of this glass is very high, ***so these tubes must absolutely never be used for variable temperature work.***

These tubes are acceptable (but not recommended) for routine work on the 300 MHz instrument. However, they should be checked for proper fit in the spinner turbine before use. They should not be used on the 500 MHz and 600 MHz instruments. Of these tubes, the Norell XR55 tubes seem to be a bit better than the rest.

# Wilmad 506PP and 507PP tubes (and equivalents, ~ $12 - $15 each)

These tubes are made from Pyrex, and are the preferred tubes for use on the 300 MHz instrument. They are acceptable for use on the 500 MHz and 600 MHz instruments. However, there may be a slight (but probably unnoticeable) decrease in resolution.

# Wilmad 528PP and 535PP tubes (and equivalents, ~ $25 - $30 each)

These are premium (expensive) Pyrex tubes, and are the preferred tubes for use on the 500 MHz and 600 MHz instruments. There are no advantages to using these tubes on the 300 MHz instrument.

# Wilmad 545PP (~ $55 each)

These are an extremely thin walled tube for use on higher field instruments. They provide about a 12% increase in sensitivity over a regular tube. They are more fragile than regular tubes and should not be used with the sample changer on the 300 MHz instrument.

# Shigemi tubes (~ $300 each)

These are special tubes with a plug of susceptibility matched glass at the bottom of the tube and moveable plug of susceptibility matched glass that goes in from the top. These tubes allow you to use a smaller sample volume (typically 250 μl) thus concentrating your sample and maximizing sensitivity. The glass must be matched to the solvent in use. For example, there are different tubes for CDCl3 and D2O. You also need different tubes for Bruker and Varian/Agilent spectrometers. These tubes are ***very*** expensive and are most commonly used for protein NMR spectroscopy. An alternative, if solubility is not an issue, is to use 1.7 mm tubes in the 1.7 mm probe on the AV III 500.

# 1.7 mm tubes ($3 each) Avance III 500 only

These are special tubes for use with the 1.7 mm microprobe on the AV III 500 instrument. These tubes are disposable, and can be purchased from the NMR lab for $3.00 each. These tubes are recommended for extremely small samples (< 1mg) and require about 40 μl of deuterated solvent. Special tools (available in the NMR lab) are required for sample handling and closing of the sample tube. To recover your sample from these tubes you must cut the tube open.