The Resonator

NMR - MRI Newsletter **Special ENC Edition**

DEAR COLLEAGUE,

It seems strange to realize that the last conference we traveled to was the ENC in March 2020. It felt like we went home to a different world.

While dealing with Covid here in South Carolina, not traveling, and with our work interrupted at times by Covid's rough hand, important things have been happening at Doty Scientific.

We published a paper in JMRO "***New insights from broadband simulations into small over-moded smooth and corrugated terahertz waveguides and transitions for NMR-DNP"***, available here https://doi.org/10.1016/j.jmro.2020.100009; and we received an NIH grant to continue our work on microwave waveguides.

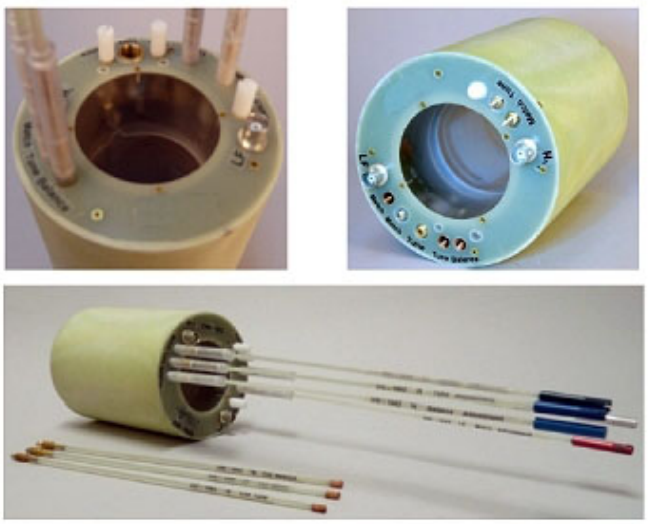
In This Issue

We purchased and had installed a new JEOL 500MHz NMR Console, and there were new probe developments. ***Please join our ENC webinar for more information.***

We miss seeing you in person. We hope you are safe and well. David and Judy Doty

Dual Frequency MRI Coils ^{1}H/X and ^{1}H/^{19}F

Dual-frequency MR Coils enable MR spectroscopy and imaging techniques, including hyperpolarized nuclei. Detailed full-wave simulations ensure the highest sensitivity, homogeneity, and isolation between channels. B1 field maps and SAR maps included with each coil. Flexible design can be customized for your application and MR system.



65 x 52 mm ^{1}H/X Dual Frequency Coils

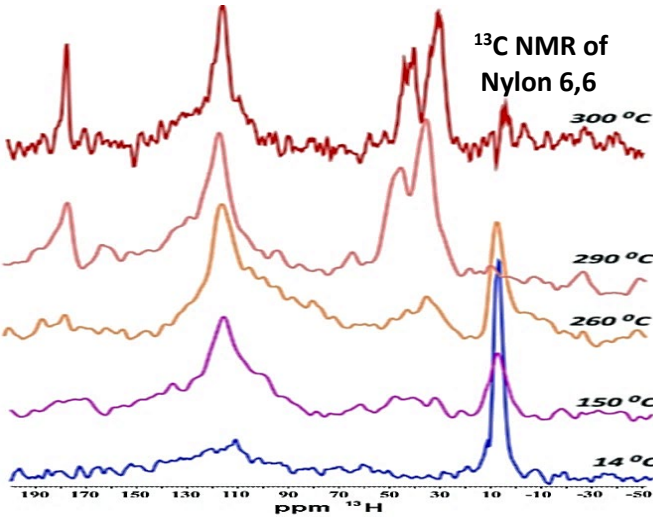
- **Efficient, easy to tune and match over a broad range of sample loadings.**
- **Each channel for TxRx.**
- **For observe / decouple – with both channels simultaneously.**
- **For interleaved acquisitions - with each channel used sequentially.**
- **Robust design, mechanical stability.**

Examples of recent dual-frequency coils we have supplied *(ID x RF length)*:

- 65 x 52 mm, ^{1}H/X, *(X=^{13}C, ^{15}N),* @ 3 T; 1.5 T; 1 T; 0.5 T; and 0.3 T.
- 45 x 36 mm, ^{1}H/X *(X=^{31}P, ^{13}C),* @ 7 T.
- 38 x 34 mm, ^{1}H/X, *(X=^{31}P, ^{13}C),* @ 9.4 T.
- 25 x 22 mm, ^{1}H/X, *(X=^{31}P, ^{13}C),* @ 9.4 T.
- 25 x 22 mm, ^{1}H/^{13}C, @ **14.1 T.**
- **200 x 160 mm**, ^{1}H/^{23}Na, @ **4.7 T.**
- 38 x 55 mm, **^{1}H/^{19}F**, @ 7 T.
- Surface Coil 16 mm, ^{1}H/^{15}N, @ 7 T.

High Temperature
HR Liquids and PFG Probes

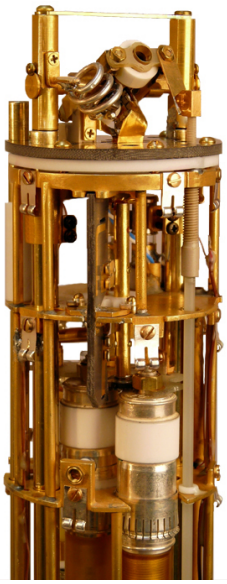
- **Extended Temperature (XVT) to +300 °C for liquids including macromolecules**
- **With water cooled Z-gradient.**
- **Pulsed gradient >1000 G/cm.**
- **5 mm sample coil**
- **Many tuning options: H/X/lock, H-F/X/lock, H/C/N/lock, H/F/X/lock.**



Spectra taken on a NB, 600 MHz, 5mm, Doty high temperature PFG probe, ^{1}H-^{19}F/X/^{2}H Lock, XVT -120°C to +300°C, water-cooled 20-40c Z Gradient

The peak near 10 ppm is from the silicone oil which surrounded a nylon screw. The oil was displaced by the nylon when it melted above 264C (and ran down, filling the sample window), and then the narrowed lines from the liquid nylon become prominent.

High Temperature
Ultra-range MAS probes



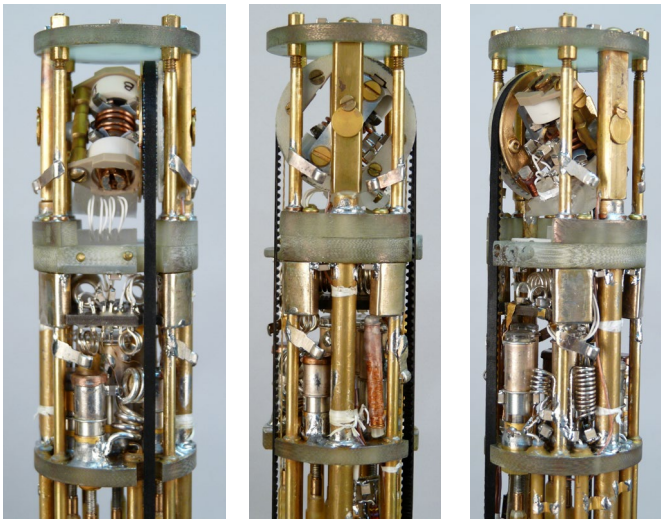
- **Widebore Ultra-Range – Now up to +500°C**
- **Broad Temperature Range** -100 °C to **+500 °C**
- **Broad Tuning Range** with tuning inserts ^{31}P to ^{103}Rh
  Double-Tuned ^{1}H/X or Triple-Tuned ^{1}H/X/Y
- 300 MHz to 700 MHz
- 5 mm spinner
- 10 kHz MAS from 200°C to +500°C

produced ***The Resonator***, Doty Scientific's newsletter is a few times each year. If you enjoy this newsletter and wish to receive our news in the future, please click newsletter sign-up. That will take you to the sign-up page on our website.

Under Development:
A New Look at Switched Angle Spinning – SAS with PFG

Left: Photo showing the new, completed, triple-resonance SAS probe (on the right) and the 3 axis PFG gradient coil. The gradient coil fits inside standard WB high-field magnet shim bores (73 mm ID). The SAS probe (46.5 mm OD) slides inside the gradient coil.

Right: Three views of the Doty triple-resonance 500 MHz SAS Probe

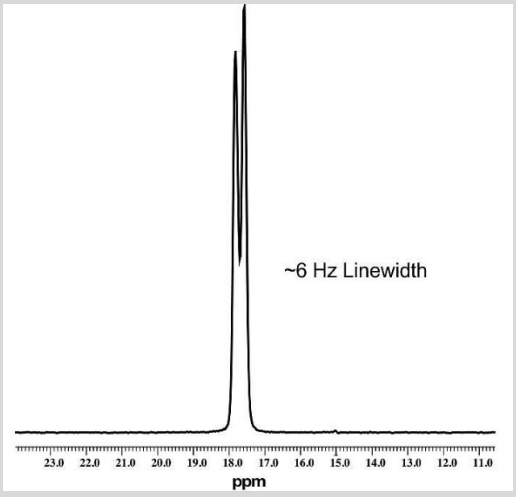


The Doty triple-resonance 500 MHz SAS Probe

Given the apparent complexity around the sample, resolution in a SAS might be an issue. Below we show that is not an issue.

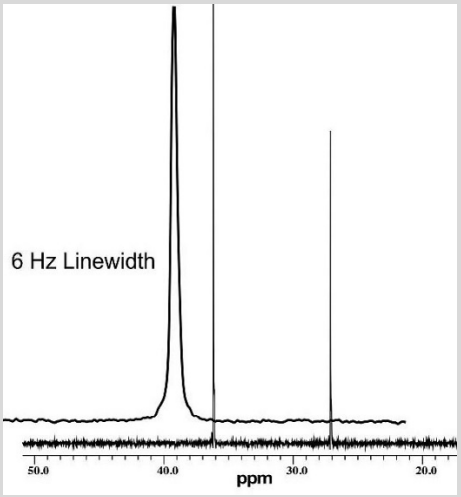
Resolution in the Doty SAS Probe

The Chemicl Shift of 0.2735 ppm Corresponds to a Shift of ~14 Hz.



^{15}N of ^{15}N labeled (100%) Ammonium Sulfate, spinning a 5 kHz illustrating the crystallographic nonequivalent sites, 4 Scans

Expansion of the Deshielded Resonance of Adamantane



^{13}C NMR of Adamantane at 11.7 T spinning at 5.2 kHz, 4 scans

Summary of the resolution in the 4 mm Doty SAS probe. In the case of 15N resolution (6Hz) is sufficient to resolve the nonequivalent sites in ammonium sulfate. In the case of adamantane the resolution is ~6 Hz.